



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 133273**

**TO: Ben Sackey**  
**Location: rem/5b31/5c18**  
**Art Unit: 1626**  
**Wednesday, September 22, 2004**

**Case Serial Number: 10/786992**

**From: Noble Jarrell**  
**Location: Biotech-Chem Library**  
**Rem 1B71**  
**Phone: 272-2556**

**Noble.jarrell@uspto.gov**

### **Search Notes**

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Noble

Access DB# 133273

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN JACKET Examiner #: 73489 Date: 9/21/04  
 Art Unit: 1620 Phone Number: 302-0704 Serial Number: 10/786,992  
 Mail Box and Bldg/Room Location: REM 5 B 31 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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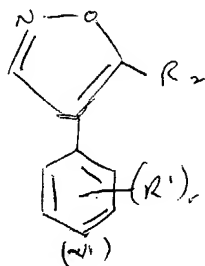
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Convergent Synthesis of alpha -aryl-beta-ketonitriles  
 Inventors (please provide full names): Jig cheng Zhou et al.

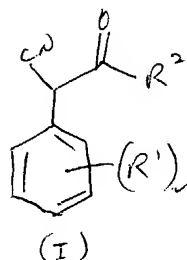
Earliest Priority Filing Date: 4/3/98

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

compos of claims 10 and 11 respectively



claim 10 substituents  
 are as defined in the  
 claim.



(I)  
 claim 11 substituents are  
 as defined in the claim.

Thanks

## STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>Noble</u>	NA Sequence (#) _____	STN <u>685</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>1</u>	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: <u>9/22/04</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>30</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: <u>30</u>	Other _____	Other (specify) _____

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 FILE 'REGISTRY' ENTERED AT 14:39:57 ON 22 SEP 2004  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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Property values tagged with IC are from the ZIC/VINITI data file  
 provided by InfoChem.

STRUCTURE FILE UPDATES: 21 SEP 2004 HIGHEST RN 749178-43-6  
 DICTIONARY FILE UPDATES: 21 SEP 2004 HIGHEST RN 749178-43-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

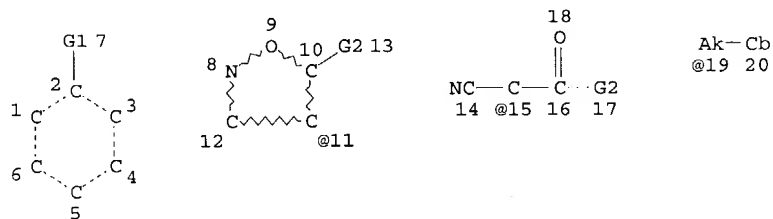
Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d que stat 19

L7 STR



Ak-OH @21 22      Ak-X @23 24

VAR G1=11/15  
 VAR G2=H/AK/CB/19/21/23  
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 1 8  
 NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE  
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FILE 'REGISTRY' ENTERED AT 13:07:11 ON 22 SEP 2004

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 TRA L1 1- RN : 13 TERMS

L3 FILE 'REGISTRY' ENTERED AT 13:07:14 ON 22 SEP 2004  
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 SEL AN  
 EDIT E1-E154 /AN /OREF

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 E ZHOU JIACHENG/AU  
 L15 28 E3  
 E OH L/AU  
 L16 10 E16-17  
 E MA P/AU  
 L17 97 E3-14  
 E MA PHILIP/AU  
 L18 39 E3-5  
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 L21 10 L13 AND L19  
 L22 9 L21 NOT L20  
 L23 1804 L13 NOT L20  
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 L25 848 L9 (L) PREP+NT/RL  
 L26 641 L25 AND (PY<=1998 OR AY<=1998 OR PRY<=1998 OR PD<19980403 OR AD  
 L27 124 L26 AND P/DT AND US/PC  
 L28 60 L26 AND P/DT AND US/PC.B

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FILE 'HCAPLUS' ENTERED AT 14:40:22 ON 22 SEP 2004  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 22 Sep 2004 VOL 141 ISS 13  
 FILE LAST UPDATED: 21 Sep 2004 (20040921/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all fhitr 120 tot

L20 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:368618 HCAPLUS  
 DN 138:368624  
 ED Entered STN: 14 May 2003  
 TI Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles.  
 IN Zhou, Jiacheng; Oh, Lynette May; Ma, Philip  
 PA Bristol-Myers Squibb Pharma Company, USA  
 SO U.S., 20 pp.  
 CODEN: USXXAM

Searched by Noble Jarrell

DT Patent  
 LA English  
 IC ICM C07D295-033  
 ICS C07D241-04; C07D211-60; C07D207-06; C07C253-12  
 NCL 544059000; 558355000; 558309000; 544159000; 544163000; 544399000;  
 546230000; 548579000  
 CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 FAN.CNT 2

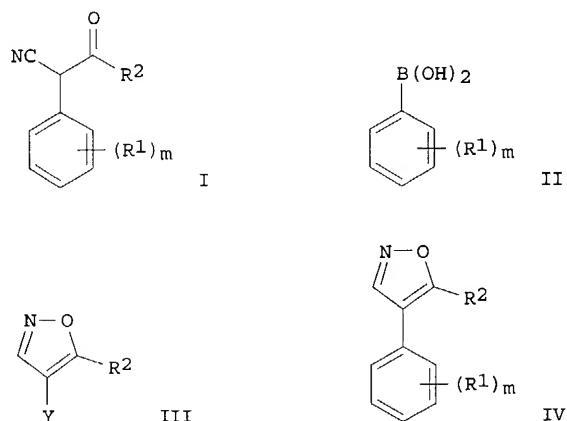
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	US 6727360	B2	20040427		
	US 2004171829	A1	20040902	US 2004-786992	20040225
PRAI	US 1998-80680P	P	19980403		
	US 1999-282508	A3	19990331		
	US 2000-610819	A3	20000706		
	US 2003-387759	A3	20030313		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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	NCL	544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000
US 6562965	ECLA	C07C255/41
US 2003208068	ECLA	C07C253/00; C07C255/41; C07D201/08; C07D261/08; C07D261/10B

OS CASREACT 138:368624; MARPAT 138:368624

GI



AB .alpha.-Aryl-.beta.-ketonitriles [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], which serve as synthetic intermediates in the preparation of biol. important mols. such as corticotropin releasing factor (CRF) receptor antagonists, were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO<sub>3</sub>, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H<sub>2</sub>O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.

ST arylketonitrile convergent synthesis; nitrile arylketo convergent synthesis

IT Nitriles, preparation  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (oxo; convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 72287-26-4, [1,1'-Bis(diphenylphosphino)ferrocene]palladium dichloride

RL: CAT (Catalyst use); USES (Uses)  
 (convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
 arylboronic acids and isoxazoles)

IT 246023-57-4P 246023-58-5P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
 arylboronic acids and isoxazoles)

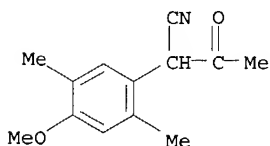
IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole  
 27060-75-9, 4-Bromo-3-methylanisole  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
 arylboronic acids and isoxazoles)

IT 7064-37-1P, 4-Bromo-5-Methylisoxazole 7064-38-2P, 4-Iodo-5-  
 methylisoxazole 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P,  
 4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-  
 methoxybenzeneboronic acid 246023-55-2P 246023-56-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
 arylboronic acids and isoxazoles)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) de Munno, A; J Chem Soc, Perkin Trans 2 1977, 9, P1121 HCAPLUS  
 (2) Dominguez, E; J Org Chem 1966, V61, P5435  
 (3) Hiroyuki, Y; Chemical Abstracts 1959, V53(22)  
 (4) Hiroyuki, Y; Yakugaku Zasshi 1959, V79, P623  
 (5) Labadie, S; Synthetic Communications 1994, V24(5), P709 HCAPLUS  
 (6) Larock, R; Comprehensive organic transformations 1970, P57  
 (7) Mitchell, R; J Org Chem 1979, V44, P4733 HCAPLUS  
 (8) Olah, G; J Org Chem 1993, V58, P3894  
 (9) Olah, G; Journal of Organic Chemistry 1993, V58, P3194 HCAPLUS  
 (10) Rouiller, C; Heterocyclic Compounds-More than One Hetero Atom 1962, P3465  
 (11) Sakakibara, T; Chem Express 1989, V4, P85 HCAPLUS  
 (12) Sumimoto; US 4797492 A 1989 HCAPLUS  
 (13) Zhou; US 6107508 A 2000 HCAPLUS

IT 246023-57-4P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
 arylboronic acids and isoxazoles)

RN 246023-57-4 HCAPLUS  
 CN Benzeneacetoneitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA  
 INDEX NAME)



L20 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:659354 HCAPLUS  
 DN 131:286268  
 ED Entered STN: 15 Oct 1999  
 TI Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic  
 acids and isoxazoles.  
 IN Zhou, Jicheng; Oh, Lynette May; Ma, Philip  
 PA Du Pont Pharmaceuticals Company, USA  
 SO PCT Int. Appl., 64 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07C253-00  
 CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9951568	A2	19991014	WO 1999-US6822	19990329
WO 9951568	A3	19991118		

W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ,  
 PL, RO, SG, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE

CA 2326846	AA	19991014	CA 1999-2326846	19990329
AU 9932135	A1	19991025	AU 1999-32135	19990329
BR 9909427	A	20001121	BR 1999-9427	19990329
EP 1066250	A2	20010110	EP 1999-914246	19990329

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SI, LT, LV, FI, RO

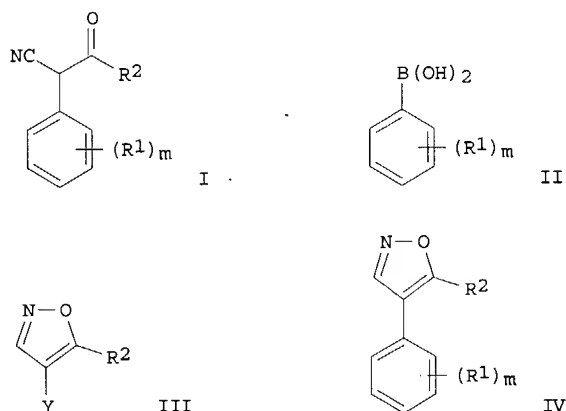
EE 200000580	A	20020215	EE 2000-580	19990329
JP 2002510670	T2	20020409	JP 2000-542290	19990329
US 6107508	A	20000822	US 1999-282508	19990331
ZA 2000004654	A	20011011	ZA 2000-4654	20000905
NO 2000004956	A	20001101	NO 2000-4956	20001002

PRAI US 1998-80680P	P	19980403
WO 1999-US6822	W	19990329

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 9951568	ICM	C07C253-00
WO 9951568	ECLA	C07C253/00; C07D201/08
OS	CASREACT	131:286268; MARPAT 131:286268
GI		



AB Title compds. [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO<sub>3</sub>, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H<sub>2</sub>O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.

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RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

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IT 246023-57-4P 246023-58-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole 7064-37-1,

4-Bromo-5-Methylisoxazole 7064-38-2, 4-Iodo-5-methylisoxazole

27060-75-9, 4-Bromo-3-methylanisole

RL: RCT (Reactant); RACT (Reactant or reagent)

(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
arylboronic acids and isoxazoles)

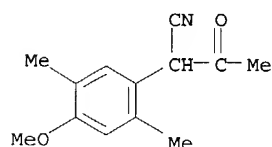
IT 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P,  
4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-  
methoxybenzeneboronic acid 246023-55-2P 246023-56-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
arylboronic acids and isoxazoles)

IT 246023-57-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
(Preparation)(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from  
arylboronic acids and isoxazoles)

RN 246023-57-4 HCAPLUS

CN Benzeneacetone nitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA  
INDEX NAME)

=&gt; d all fhitrstr l22 tot

L22 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:813420 HCAPLUS

DN 135:344507

ED Entered STN: 08 Nov 2001

TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing  
factor (CRF) antagonists

IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios

PA Dupont Pharmaceuticals Company, USA

SO U.S., 57 pp., Cont.-in-part of U.S. Ser. No. 899,242.

CODEN: USXXAM

DT Patent

LA English

IC A61K031-535; C07D487-04

NCL 514246000

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 2, 63

FAN.CNT 5

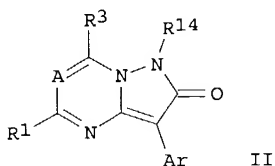
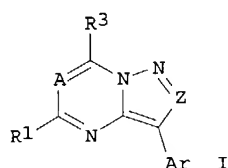
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	ZA 9706603	A	19990125	ZA 1997-6603	19970724
	US 6136809	A	20001024	US 1998-14999	19980128
	LT 4680	B	20000725	LT 1999-8	19990125
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	AU 748818	B2	20020613		
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	JP 2002501922	T2	20020122	JP 2000-529335	19990128
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	EP 1344779	A1	20030917	EP 2003-75887	19990128
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Searched by Noble Jarrell

AT 264860	E	20040515	AT 1999-904382	19990128
TW 520372	B	20030211	TW 1999-88102636	19990223
US 2003008885	A1	20030109	US 2001-930782	20010816
PRAI US 1996-23290P	P	19960724		
US 1997-899242	A2	19970723		
US 1998-14734	A	19980128		
US 1998-15001	A	19980128		
US 1998-15002	A	19980128		
EP 1999-904382	A3	19990128		
WO 1999-US1824	W	19990128		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6313124	IC	A61K031-535IC C07D487-04
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EP 1344779	ECLA	C07D487/04; C07D487/04
US 2003008885	ECLA	C07D487/04; C07D487/04; C07D487/04
OS MARPAT 135:344507		
GI		



- AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists (no data) which are useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl) [1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline, followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dichlorophenyl) [1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxy-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].
- ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor antagonist azolotriazine azolopyrimidine prepn
- IT Corticotropin releasing factor receptors  
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)
- IT 202578-49-2P 202579-55-3P 202579-56-4P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)
- IT 202578-50-5P 202578-51-6P 202578-52-7P 202578-53-8P 202578-54-9P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 105-53-3, Diethyl malonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1000-84-6 1445-45-0, Trimethyl orthoacetate 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetone nitrile 78531-29-0 202580-72-1 202580-73-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

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202580-62-9P, 5-Amino-4-(2,4-dimethylphenyl)-3-methylpyrazole  
202580-64-1P 202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

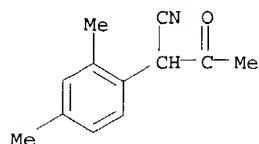
RE.CNT 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD

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 IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing  
 factor (CRF) antagonists)  
 RN 202580-61-8 HCAPLUS  
 CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:618005 HCAPLUS  
 DN 135:195579  
 ED Entered STN: 24 Aug 2001  
 TI Preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of  $\alpha$ .beta. protein production  
 IN Olson, Richard E.; Maduskuie, Thomas P.; Thompson, Lorin Andrew; Tebben, Andrew J.; Wang, Nenghui; Deng, Wei; Liu, Hong  
 PA Dupont Pharmaceuticals Company, USA  
 SO PCT Int. Appl., 236 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D487-04  
 ICS C07D471-04; C07D471-08; C07D243-24; A61K031-55; A61K031-551; A61K031-5513; A61K031-5517; A61P025-28; C07D487-04; C07D223-00; C07D209-00; C07D471-04; C07D223-00; C07D221-00; C07D471-08; C07D223-00; C07D221-00; C07D487-04; C07D223-00

CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

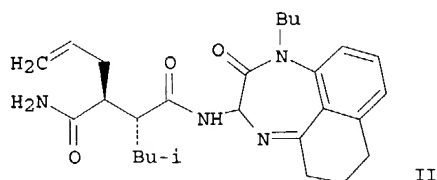
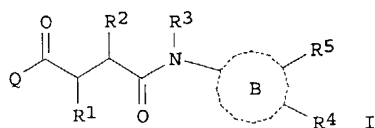
## FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001060826	A2	20010823	WO 2001-US5236	20010216
WO 2001060826	A3	20020117		
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 2002055501	A1	20020509	US 2001-788227	20010216
US 6525044	B2	20030225		
EP 1261610	A2	20021204	EP 2001-914400	20010216
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JP 2003523345	T2	20030805	JP 2001-560210	20010216
PRAI US 2000-183186P	P	20000217		
WO 2001-US5236	W	20010216		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001060826	ICM	C07D487-04
	ICS	C07D471-04; C07D471-08; C07D243-24; A61K031-55; A61K031-551; A61K031-5513; A61K031-5517; A61P025-28; C07D487-04; C07D223-00; C07D209-00; C07D471-04; C07D223-00; C07D221-00; C07D471-08; C07D223-00; C07D221-00; C07D487-04; C07D223-00
US 2002055501	ECLA	C07D243/24; C07D401/06; C07D471/04; C07D471/04; C07D471/06; C07D471/08; C07D487/04; C07D487/04; C07D487/06; C07D087/06

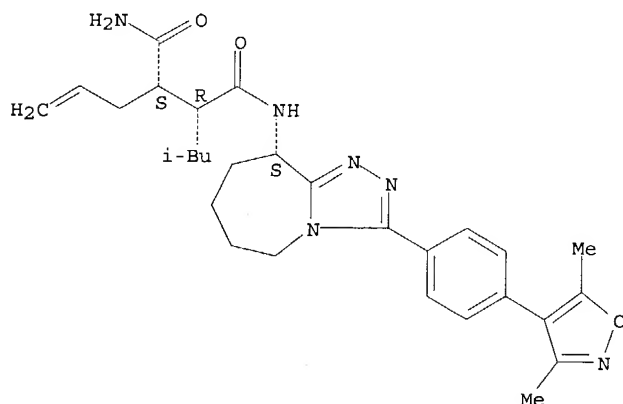
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 GI



- AB Synthesis of succinoylamino carbocycles and heterocycles (I) [Q = (un)substituted OH, NH<sub>2</sub>; R<sub>1</sub> = (un)substituted alkyl, alkenyl; R<sub>2</sub> = (un)substituted alkyl; R<sub>3</sub> = H, alkyl; R<sub>4</sub> = (un)substituted aryl; R<sub>5</sub> = (un)substituted OH, (un)substituted CONH<sub>2</sub>, (un)substituted alkyl; B = nitrogen heterocycle fused by one or more (un)substituted (un)saturated carbocyclic or heterocyclic rings] having drug and bio-affecting properties, their pharmaceutical compns. and methods of use is disclosed. Thus, (II) was prepared by amidation of 2-amino-3-oxo-2,3,4,8,9,10-hexahydronaphtho[1,8-e]diazepine with tert-Bu (2R,3S)-3-allyl-2-isobutylsuccinic acid followed by aminolysis and butylation. II inhibits production of .beta.-amyloid protein with an IC<sub>50</sub> < 100.upsilon.M in an immunopptn. assay using N9 cells characterized for expression of exogenous amyloid precursor protein. These novel compds. inhibit the processing of amyloid precursor protein and, more specifically, inhibit the production of A.beta.-peptide, thereby acting to prevent the formation of neurol. deposits of amyloid protein. More particularly, the present invention relates to the treatment of neurol. disorders related to .beta.-amyloid production such as Alzheimer's disease and Down's Syndrome.
- ST amyloid protein inhibitor succinoylamino carbocycle heterocycle
- IT Anti-Alzheimer's agents  
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT Amyloid  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT Down's syndrome  
(treatment of; preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 158736-49-3, .beta. Secretase 338454-52-7, .gamma. Secretase  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(method for inhibition of; preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 356040-26-1P 356040-27-2P 356040-34-1P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 356040-12-5P 356040-13-6P 356040-14-7P 356040-15-8P 356040-16-9P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 356040-61-4P  
RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

- IT 356040-76-1P 356040-77-2P  
 RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PREP (Preparation); PROC (Process)  
 (preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 62-53-3, Aniline, reactions 74-88-4, Iodomethane, reactions 75-31-0, Isopropylamine, reactions 98-80-6, Phenylboronic acid 100-46-9, Benzylamine, reactions 542-69-8, Butyl iodide 1210-35-1, Dibenzosuberone 1679-18-1, 4-Chlorophenylboronic acid 2217-41-6, 5,6,7,8-Tetrahydro-1-naphthylamine 2393-23-9, 4-Methoxybenzylamine 3218-02-8, Cyclohexanemethanamine 5071-96-5, 3-Methoxybenzylamine 5392-81-4 5933-32-4 16114-47-9 16947-84-5 33244-57-4 54631-81-1 55401-97-3, 2-(Bromomethyl)pyridine 65365-28-8, D-Proline methyl ester hydrochloride 76944-95-1 90600-20-7 98437-24-2 114715-38-7, (S)-3-Amino-1-benzylpyrrolidine 114715-39-8, (R)-3-Amino-1-benzylpyrrolidine 124676-19-3 126544-38-5 148415-75-2 204326-24-9 219615-42-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 1785-74-6P 6272-18-0P 7005-53-0P 39115-96-3P 109953-95-9P  
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 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- IT 356040-33-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)
- RN 356040-33-0 HCAPLUS
- CN Butanediamide, N1-[(9S)-3-[4-(3,5-dimethyl-4-isoxazolyl)phenyl]-6,7,8,9-tetrahydro-5H-1,2,4-triazolo[4,3-a]azepin-9-yl]-2-(2-methylpropyl)-3-(2-propenyl)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:131201 HCAPLUS  
 DN 134:178572  
 ED Entered STN: 22 Feb 2001  
 TI Preparation of azolo triazines and pyrimidines as corticotropin releasing factor (CRF) antagonists  
 IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios  
 PA Dupont Pharmaceuticals Co., USA

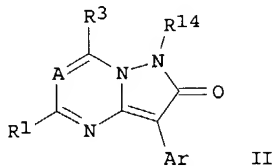
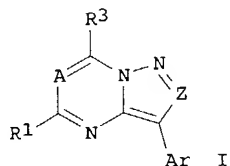
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 ICS C07D251-72; A61K031-53  
 NCL 514246000  
 CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 2, 63  
 FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6191131	B1	20010220	US 1998-15002	19980128
	US 6124289	A	20000926	US 1997-899242	19970723
	ZA 9706603	A	19990125	ZA 1997-6603	19970724
	US 6136809	A	20001024	US 1998-14999	19980128
	LT 4680	B	20000725	LT 1999-8	19990125
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
	WO 9938868	A1	19990805	WO 1999-US1824	19990128
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9924787	A1	19990816	AU 1999-24787	19990128
	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128
	EP 1049699	B1	20040421		
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	BR 9908206	A	20001205	BR 1999-8206	19990128
	JP 2002501922	T2	20020122	JP 2000-529335	19990128
	NZ 505079	A	20030829	NZ 1999-505079	19990128
	EP 1344779	A1	20030917	EP 2003-75887	19990128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	AT 264860	E	20040515	AT 1999-904382	19990128
	TW 520372	B	20030211	TW 1999-88102636	19990223
	US 6358950	B1	20020319	US 2000-696759	20001026
PRAI	US 1996-23290P	P	19960724		
	US 1997-899242	A2	19970723		
	US 1998-14734	A	19980128		
	US 1998-15001	A	19980128		
	US 1998-15002	A	19980128		
	EP 1999-904382	A3	19990128		
	WO 1999-US1824	W	19990128		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6191131	ICM	C07D487-04
	ICS	C07D251-72; A61K031-53
	NCL	514246000
EP 1344779	ECLA	C07D487/04; C07D487/04
OS	MARPAT	134:178572
GI		



AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alk(en/yn)yl, halo, etc.; R1, R2 = H, alk(en/yn)yl, halo, etc.; R3 = H, SH, aryl, etc.; R14 = (un)substituted alk(en/yn)yl, cycloalkyl(alkyl)], useful in treating CRF-related disorders, particularly anxiety, depression, and other psychiatric, neurol. disorders as well as treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. For

instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-2,5-dimethyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl<sub>3</sub> and PhNEt<sub>2</sub> to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound I [A = CH; R<sub>1</sub> = Me; R<sub>3</sub> = NHCH<sub>2</sub>Et; Z = CMe; Ar = 2-Cl-4-MeC<sub>6</sub>H<sub>3</sub>]. The compds. I are effective at 0.002-200 mg/kg/day.

ST azolo triazine pyrimidine prepn formulation CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine prepn formulation CRF receptor antagonist; azolopyrimidine prepn formulation CRF receptor antagonist  
IT Antidepressants  
Anxiolytics

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)  
IT Corticotropin releasing factor receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)  
IT 202578-49-2P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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	202578-62-9P	202578-63-0P	202578-64-1P	202578-65-2P	202578-66-3P
	202578-67-4P	202578-68-5P	202578-69-6P	202578-70-9P	202578-71-0P
	202578-72-1P	202578-73-2P	202578-74-3P	202578-75-4P	202578-76-5P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)  
IT 234773-54-7P 234773-56-9P 234773-58-1P 234773-60-5P 234773-62-7P

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234774-14-2P	234774-15-3P	234774-16-4P	234774-17-5P	234774-18-6P
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234774-44-8P	234774-45-9P	234774-46-0P	234774-47-1P	234774-48-2P
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234776-03-5P	234776-04-6P	234776-05-7P	234776-06-8P	234776-07-9P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT	234776-17-1P	234776-18-2P	234776-19-3P	234776-20-6P	234776-21-7P
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	234776-28-4P	234776-29-5P	234776-30-8P	234776-31-9P	234776-32-0P
	234776-33-1P	234776-34-2P	234776-35-3P	234776-36-4P	234776-37-5P
	234776-38-6P	234776-39-7P	234776-40-0P	234776-41-1P	234776-42-2P
	234776-43-3P	234776-44-4P	234776-45-5P	234776-46-6P	234776-47-7P
	234776-48-8P	234776-49-9P	234776-50-2P	234776-51-3P	234776-52-4P
	234776-53-5P	234776-54-6P	234776-55-7P	234776-56-8P	234776-57-9P
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	234776-63-7P	234776-64-8P	234776-65-9P	234776-66-0P	234776-67-1P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT	105-53-3, Diethyl malonate	105-58-8, Diethyl carbonate	141-97-9, Ethyl acetate	616-24-0, 3-Pentylamine	622-79-7, Benzyl azide
	1445-45-0, Trimethyl orthoacetate	2208-07-3	34688-71-6,		
	2,4,6-Trimethylbenzyl cyanide	68429-53-8,	2,4-Dimethylphenylacetone	nitrile	
	78531-29-0	202580-72-1	202580-73-2	326821-97-0	

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 1000-84-6P 202580-61-8P 202580-62-9P 202580-64-1P  
 202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RE.CNT 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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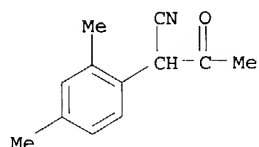
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(Reactant or reagent)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RN 202580-61-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:307132 HCAPLUS

DN 132:321873

ED Entered STN: 12 May 2000

TI Azolo triazines and pyrimidines useful as corticotropin releasing factor (CRF) antagonists

IN Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios

PA DuPont Pharmaceuticals Co., USA

SO U.S., 86 pp., Cont.-in-part of U.S. Ser. No. 899,242.

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K031-505

ICS C07D487-04

NCL 514258000

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 2

FAN.CNT 5

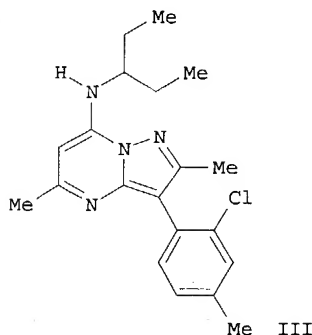
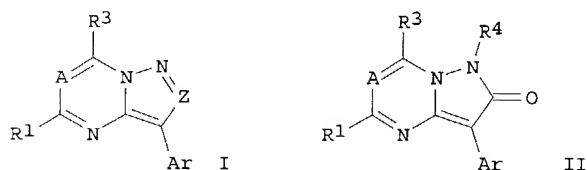
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	ZA 9706603	A	19990125	ZA 1997-6603	19970724
	US 6136809	A	20001024	US 1998-14999	19980128
	LT 4680	B	20000725	LT 1999-8	19990125
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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	AU 748818	B2	20020613		
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Searched by Noble Jarrell

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 AT 264860 E 20040515 AT 1999-904382 19990128  
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## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6060478	ICM	A61K031-505
	ICS	C07D487-04
	NCL	514258000
US 6060478	ECLA	C07D487/04; C07D487/04; C07D487/04
EP 1344779	ECLA	C07D487/04; C07D487/04
OS MARPAT 132:321873		
GI		



AB Corticotropin releasing factor (CRF) antagonists (no data) of formulas I and II are disclosed [wherein A = N or CR; Z = N or CR<sub>2</sub>; Ar = (un)substituted Ph, naphthyl, pyridyl, pyrimidinyl, indanyl, tetralinyl, addnl. selected heterocycles; R = H, alk(en/yn)yl, cycloalkyl(alkyl), halo, cyano, haloalkyl; R<sub>1</sub>, R<sub>2</sub> = H, groups listed for R, NH<sub>2</sub> or derivs., OH or derivs., SH or derivs., addnl. substituted alkyls; R<sub>3</sub> = H, OH or derivs., SH or derivs., acyl, CO<sub>2</sub>H or esters, NH<sub>2</sub> or derivs., aryl, heteroaryl, alk(en/yn)yl, etc.; R<sub>4</sub> = (un)substituted alk(en/yn)yl or cycloalkyl(alkyl)]. The compds. are of use in the treatment of CRF-related disorders, particularly anxiety and depression, as well as other psychiatric, neurol., immunol., cardiovascular, and psychopathol. disorders. For instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-5-methyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl<sub>3</sub> and PhNET<sub>2</sub> to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound III.

ST azolo triazine pyrimidine prepn CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine azolopyrimidine prepn CRF receptor antagonist

IT Drugs  
(gastrointestinal; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Intestine, disease  
(irritable bowel syndrome, treatment; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Anti-inflammatory agents  
Antidepressants  
Anxiolytics  
Cardiovascular agents  
Immunomodulators  
Nervous system agents  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Corticotropin releasing factor receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 9015-71-8, Corticotropin releasing factor  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 105-53-3, Diethyl malonate 105-58-8 141-78-6, Acetic acid ethyl ester, reactions 141-97-9 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1445-45-0, Trimethyl orthoacetate 2208-07-3 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetone nitrile 78531-29-0, 1,3-Dimethoxy-2-aminopropane 202580-72-1 202580-73-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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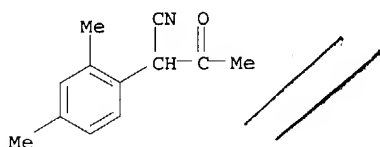
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD

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 IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (intermediate; preparation of azolo-fused triazines and pyrimidines as CRF  
 antagonists)  
 RN 202580-61-8 HCAPLUS  
 CN Benzeneacetoneitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:125866 HCAPLUS  
 DN 132:231516  
 ED Entered STN: 24 Feb 2000  
 TI The discovery of 4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)-pyrazolo-[1,5-a]-pyrimidine: a corticotropin-releasing factor (hCRF1) antagonist  
 AU Gilligan, Paul J.; Baldauf, Caryn; Cocuzza, Anthony; Chidester, Dennis; Zaczek, Robert; Fitzgerald, Lawrence W.; McElroy, John; Smith, Mark A.; Shen, H.-S. L.; Saye, Jo Anne; Christ, David; Trainor, George; Robertson, David W.; Hartig, Paul  
 CS Chemical and Physical Sciences Department, Experimental Station, DuPont Pharmaceuticals Co., Wilmington, DE, 10880-0500, USA  
 SO Bioorganic & Medicinal Chemistry (2000), 8(1), 181-189  
 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 CC 1-3 (Pharmacology)  
 Section cross-reference(s): 28

AB Structure-activity relationship studies led to the discovery of 4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)-pyrazolo-[1,5-a]-pyrimidine (compound 11-31, DMP904), whose pharmacol. profile strongly supports the hypothesis that hCRF1 antagonists may be potent anxiolytic drugs. Compound 11-31 (hCRF1 Ki = 1.0  $\pm$  0.2 nM (n = 8)) was a potent antagonist of hCRF1-coupled adenylate cyclase activity in HEK293 cells (IC50 = 10.0  $\pm$  0.01 nM vs. 10 nM r/hCRF, n = 8);  $\alpha$ -helical CRF(9-41) had weaker potency (IC50 = 286  $\pm$  63 nM, n = 3). Analog 11-31 had good oral activity in the rat situational anxiety test; the min. ED for 11-31 was 0.3 mg/kg, orally. Maximal efficacy (approx. 57% reduction in latency time in the dark compartment) was observed at this dose. Chlordiazepoxide caused a 72% reduction in latency at 20 mg/kg, orally. CP154526-1 (30 mg/kg, orally) was inactive in this test. Compound 11-31 did not inhibit open-field locomotor activity at 10, 30, and 100 mg/kg, orally in rats. In beagle dogs, this compound (5 mg/kg, i.v., orally) afforded good plasma levels. The key i.v. pharmacokinetic parameters were t1/2, CL and Vd.ss values equal to 46.4  $\pm$  7.6 h, 0.49  $\pm$  0.08 L/kg/h and 23.0  $\pm$  4.2 L/kg, resp. After oral dosing, the mean Cmax, Tmax, t1/2 and bioavailability values were equal to 1260  $\pm$  290 nM, 0.75  $\pm$  0.25 h, 45.1  $\pm$  10.2 h and 33.1%, resp. The overall rat behavioral profile of this compound suggests that it may be an anxiolytic drug with a low motor side effect liability.

ST pyrazolopyrimidine prepn structure CRF1 receptor antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine; DMP904 anxiolytic CRF1 receptor antagonist

IT Structure-activity relationship  
 (receptor-binding; structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT Anxiolytics  
 (structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT Corticotropin releasing factor receptors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (type I; structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT 9012-42-4, Adenylate cyclase  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (anxiolytic DMP904 is antagonist of hCRF1-coupled adenylate cyclase activity in HEK293 cells)

IT 202579-74-6P  
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
 (structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT 195055-41-5 202579-58-6 202579-60-0 202579-61-1 202579-62-2  
 202579-63-3 202579-75-7 202579-85-9 202579-86-0 202579-89-3  
 202579-91-7 202579-93-9 202579-94-0 202579-95-1 202579-96-2  
 202580-25-4 202580-27-6 202580-28-7 262297-99-4 262298-00-0  
 262298-01-1  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT 202579-57-5P 202579-59-7P 202579-64-4P 202579-65-5P 202579-66-6P  
 202579-68-8P 202579-69-9P 202579-70-2P 202579-71-3P 202579-72-4P  
 202579-73-5P 202579-79-1P 202579-80-4P 202579-81-5P 202579-82-6P  
 202579-83-7P 202579-88-2P 202579-90-6P 202579-92-8P 202580-29-8P  
 262297-98-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT 616-24-0, 3-Pentylamine 52289-56-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT 246023-58-5P 262298-02-2P 262298-03-3P 262298-04-4P  
262298-05-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD

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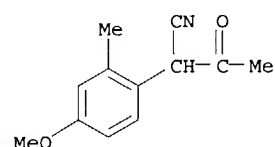
IT 246023-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

RN 246023-58-5 HCAPLUS

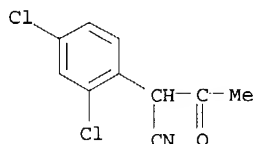
CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L22 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:60209 HCAPLUS  
 DN 132:231502  
 ED Entered STN: 26 Jan 2000  
 TI 4-(1,3-Dimethoxyprop-2-ylamino)-2,7-dimethyl-8-(2,4-dichlorophenyl)pyrazolo[1,5-a]-1,3,5-triazine: A Potent, Orally Bioavailable CRF1 Receptor Antagonist  
 AU He, Liqi; Gilligan, Paul J.; Zaczek, Robert; Fitzgerald, Lawrence W.; McElroy, John; Shen, H-S. L.; Saye, Jo Anne; Kalin, Ned H.; Shelton, Steven; Christ, David; Trainor, George; Hartig, Paul  
 CS Chemical and Physical Sciences Department, DuPont Pharmaceuticals Company, Wilmington, DE, 10880-0500, USA  
 SO Journal of Medicinal Chemistry (2000), 43(3), 449-456  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 1-3 (Pharmacology)  
 Section cross-reference(s): 28  
 AB Structure-activity studies in the pyrazolo[1,5-a]-1,3,5-triazine series led to the discovery that compound DMP696 (I) is a potent hCRF1 receptor antagonist (K<sub>i</sub> = 1.7 nM vs. 7.5 nM for .alpha.-hel-CRF(9-41), hCRF1 adenylate cyclase IC<sub>50</sub> = 82 nM vs. 286 nM for .alpha.-hel-CRF(9-41)). Compound I has excellent oral pharmacokinetic profiles in rats and dogs (37% and 50% oral bioavailabilities, resp.). This compound displays good activity in the rat situational anxiety model (MED = 3 mg/kg orally), whereas a literature standard CP154526-1 was inactive (MED > 30 mg/kg orally). Analog I reduced stereotypical mouth movements in rhesus monkeys by 50% at 21 mg/kg orally using the human intruder paradigm. Overall, the profile of pyrazolotriazine I indicates that hCRF1 receptor antagonists may be anxiolytic agents, which have reduced motor side effect profiles.  
 ST pyrazolotriazine prepn structure CRF1 receptor anxiolytic; corticotropin releasing factor receptor antagonist pyrazolotriazine  
 IT Anxiolytics  
 Drug bioavailability  
 (preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)  
 IT Structure-activity relationship  
 (receptor-binding; CRF1 receptor binding of pyrazolotriazines as potential anxiolytics)  
 IT Corticotropin releasing factor receptors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (type I; CRF1 receptor binding of pyrazolotriazines as potential anxiolytics)  
 IT 202578-53-8 202578-54-9 202578-55-0 202578-57-2 202578-58-3  
 202578-59-4 202578-60-7 202578-61-8 202578-62-9 202578-63-0  
 202578-64-1 261966-75-0  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (CRF1 receptor binding of pyrazolotriazines as potential anxiolytics)  
 IT 202578-52-7P, DMP 696  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)  
 IT 6306-60-1, 2,4-Dichlorophenylacetonitrile 78531-29-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)  
 IT 76562-15-7P 202580-70-9P 214416-40-7P 261966-73-8P  
 261966-74-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)  
 RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
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- IT 76562-15-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)
- RN 76562-15-7 HCAPLUS  
 CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dichloro- (9CI) (CA INDEX NAME)



L22 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:495296 HCAPLUS  
 DN 131:144616  
 ED Entered STN: 10 Aug 1999  
 TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists  
 IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios  
 PA Du Pont Pharmaceuticals Company, USA  
 SO PCT Int. Appl., 245 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D487-04  
 ICS A61K031-495; C07D487-04; C07D251-00; C07D231-00; C07D487-04;

C07D239-00; C07D231-00

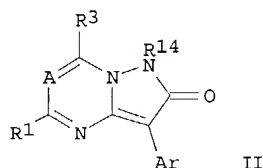
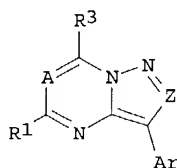
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 2, 63

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9938868	A1	19990805	WO 1999-US1824	19990128
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6060478	A	20000509	US 1998-15001	19980128
	US 6191131	B1	20010220	US 1998-15002	19980128
	US 6313124	B1	20011106	US 1998-14734	19980128
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
	AU 9924787	A1	19990816	AU 1999-24787	19990128
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	NZ 505079	A	20030829	NZ 1999-505079	19990128
	AT 264860	E	20040515	AT 1999-904382	19990128
	ZA 9900843	A	20000802	ZA 1999-843	19990203
PRAI	US 1998-14734	A	19980128		
	US 1998-15001	A	19980128		
	US 1998-15002	A	19980128		
	US 1996-23290P	P	19960724		
	US 1997-899242	A2	19970723		
	WO 1999-US1824	W	19990128		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9938868	ICM	C07D487-04
	ICS	A61K031-495; C07D487-04; C07D251-00; C07D231-00; C07D487-04; C07D239-00; C07D231-00
US 6060478	ECLA	C07D487/04; C07D487/04; C07D487/04
GI		



- AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, C1-4 alkyl, C2-4 alkenyl, etc.; R1 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R2 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists (no data) which are useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl) [1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline, followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dichlorophenyl) [1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxy-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].
- ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor antagonist azolotriazine azolopyrimidine prepn; anxiolytic azolotriazine azolopyrimidine prepn formulation; antidepressant azolotriazine azolopyrimidine prepn formulation; hypersensitivity colonic azolotriazine azolopyrimidine prepn formulation; immunol disease azolotriazine azolopyrimidine prepn formulation; cardiovascular agent azolotriazine azolopyrimidine prepn formulation
- IT Drugs  
(gastrointestinal; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other

psychiatric, neurol. disorders)

IT Intestine, disease  
(irritable bowel syndrome; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT Anti-inflammatory agents  
Antidepressants  
Anxiolytics  
Cardiovascular agents  
Immunomodulators  
Nervous system agents  
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT Mental disorder  
(treatment; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 9015-71-8, Corticotropin-releasing factor  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(antagonists; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one  
202580-62-9P 202580-63-0P 202580-64-1P 202580-66-3P 202580-68-5P  
202580-70-9P 234778-65-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 202578-49-2P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 202578-50-5P 202578-52-7P 202578-99-2P 202579-08-6P 202579-45-1P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, (2,4-Dimethylphenyl)acetonitrile 78531-29-0 202580-72-1 202580-73-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Chen, Y; WO 9533750 A 1995 HCAPLUS
- (2) Du Pont Merck Pharma; WO 9803510 A 1998 HCAPLUS
- (3) Janssen Pharmaceutica Nv; WO 9729109 A 1997 HCAPLUS
- (4) Jun, Y; WO 9635689 A 1996 HCAPLUS

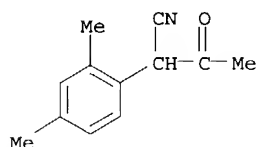
IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

RN 202580-61-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:87733 HCAPLUS

DN 128:154103

ED Entered STN: 14 Feb 1998

TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists

IN Arvanitis, Argyrios Georgious; Chorvat, Robert John

PA Du Pont Merck Pharmaceutical Co., USA

SO PCT Int. Appl., 225 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D487-04

ICS A61K031-505; C07D487-04; C07D239-00; C07D231-00; C07D487-04;  
 C07D251-00; C07D231-00; C07D487-04; C07D249-00; C07D239-00;  
 C07D487-04; C07D251-00; C07D249-00

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

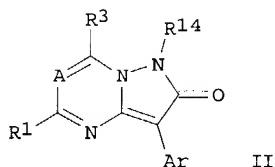
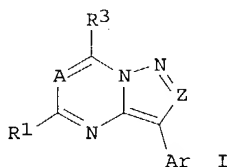
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 EP 915880 A1 19990519 EP 1997-936222 19970723  
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 CN 1104432 B 20030402  
 BR 9710544 A 19990817 BR 1997-10544 19970723  
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 TW 542827 B 20030721 TW 1997-86110640 19970725  
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 LT 4680 B 20000725 LT 1999-8 19990125  
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 AU 773039 B2 20040513 AU 2002-23236 20020312  
 CN 1388126 A 20030101 CN 2002-118589 20020425  
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 US 1996-686047 A 19960724  
 US 1997-899242 A 19970723  
 AU 1997-38942 A3 19970723  
 WO 1997-US13072 W 19970723

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9803510	ICM	C07D487-04
	ICS	A61K031-505; C07D487-04; C07D239-00; C07D231-00; C07D487-04; C07D251-00; C07D231-00; C07D487-04; C07D249-00; C07D239-00; C07D487-04; C07D251-00; C07D249-00
WO 9803510	ECLA	C07D487/04; C07D487/04; C07D487/04
OS MARPAT 128:154103		
GI		



- AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, C1-4 alkyl, C2-4 alkenyl, etc.; R1 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R2 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl) [1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dimethylphenyl) [1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxypropyl-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].
- ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor azolotriazine azolopyrimidine prepn; anxiolytic azolotriazine azolopyrimidine prepn formulation; antidepressant azolotriazine azolopyrimidine prepn formulation; hypersensitivity colonic azolotriazine azolopyrimidine prepn formulation; immunol disease azolotriazine azolopyrimidine prepn formulation; cardiovascular agent azolotriazine azolopyrimidine prepn formulation
- IT Immunity (disorder, treatment of; preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)
- IT Allergy (hypersensitivity, treatment of colonic hypersensitivity associated with psychopathol. disturbance and stress.; preparation of azolotriazines and

-pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT Antidepressants  
Anxiolytics  
Cardiovascular agents  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202578-49-2P 202579-55-3P 202579-56-4P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

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202580-03-8P 202580-04-9P 202580-05-0P 202580-06-1P 202580-07-2P  
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202580-13-0P 202580-14-1P 202580-15-2P 202580-16-3P 202580-17-4P  
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202580-23-2P 202580-24-3P 202580-25-4P 202580-26-5P 202580-27-6P  
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202580-38-9P 202580-39-0P 202580-40-3P 202580-41-4P 202580-42-5P  
202580-43-6P 202580-44-7P 202580-46-9P 202580-48-1P 202580-49-2P  
202580-50-5P 202580-51-6P 202580-52-7P 202580-53-8P 202580-54-9P  
202580-55-0P 202580-56-1P 202580-57-2P 202580-58-3P 202580-59-4P  
202580-60-7P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 9015-71-8, Corticotropin releasing factor  
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 105-53-3, Diethyl malonate 141-97-9, Ethyl acetoacetate 616-24-0,  
3-Pentylamine 622-79-7, Benzyl azide 34688-71-6, 2,4,6-Trimethylbenzyl  
cyanide 68429-53-8, 2,4-Dimethylphenylacetone nitrile 78531-29-0  
202580-72-1 202580-74-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one  
202580-62-9P 202580-64-1P 202580-65-2P 202580-66-3P 202580-68-5P  
202580-69-6P 202580-70-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD

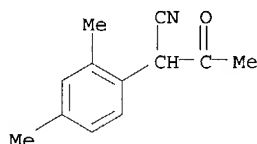
RE

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- (2) Fujisawa Pharmaceutical Co; EP 0531901 A 1993 HCAPLUS
- (3) Neurogen Corp; WO 9635689 A 1996 HCAPLUS
- (4) Otsuka Pharma Co Ltd; EP 0503099 A 1992 HCAPLUS
- (5) Otsuka Pharma Co Ltd; EP 0591528 A 1994 HCAPLUS
- (6) Otsuka Pharma Co Ltd; EP 0714898 A 1996 HCAPLUS
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- (9) Shionogi & Co Ltd; JP 61057587 A 1986 HCAPLUS
- (10) Springer, R; US 3920652 A 1975 HCAPLUS
- (11) Stanley, R; US 3995039 A 1976 HCAPLUS
- (12) Takamizawa; JP 6711753 A HCAPLUS
- (13) Takamizawa; JP 6716314 A HCAPLUS
- (14) Takamizawa; JP 7030335 A HCAPLUS

IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing  
 factor (CRF) antagonists)

RN 202580-61-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:575812 HCAPLUS

DN 99:175812

ED Entered STN: 12 May 1984

TI Herbicidal sulfonamides

IN Wolf, Anthony David; Rorer, Morris Padgett

PA du Pont de Nemours, E. I., and Co. , USA

SO Eur. Pat. Appl., 271 pp.

CODEN: EPXXDW

DT Patent

LA English

IC C07D403-00; C07D417-00; C07D413-00; A01N047-00

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 5

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 83975	A2	19830720	EP 1983-300073	19830106
	EP 83975	A3	19840801		
	EP 83975	B1	19871119		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	US 4465505	A	19840814	US 1982-428806	19821007
	US 4511392	A	19850416	US 1982-436631	19821029
	AT 30915	E	19871215	AT 1983-300073	19830106
	CA 1239929	A1	19880802	CA 1983-419031	19830106
	US 4606755	A	19860819	US 1984-685026	19841221
	US 4695311	A	19870922	US 1986-861260	19860509
	US 4810282	A	19890307	US 1987-60204	19870610
PRAI	US 1982-337932		19820107		
	US 1982-337934		19820107		
	US 1982-428806		19821007		
	US 1982-436631		19821029		
	EP 1983-300073		19830106		
	US 1984-685026		19841221		
	US 1986-861260		19860509		

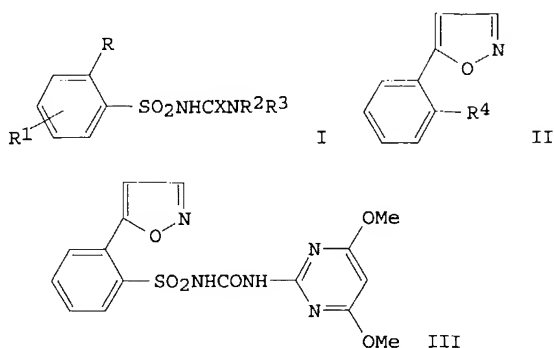
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 83975	IC	C07D403-00IC C07D417-00IC C07D413-00IC A01N047-00

OS CASREACT 99:175812

GI





AB Benzenesulfonamides I (R = azolyl, azinyl; R<sub>1</sub> = H, F, Cl, Br, Me, CF<sub>3</sub>, OMe; R<sub>2</sub> = H, Me; R<sub>3</sub> = substituted pyrimidinyl, triazinyl; X = O, S) (67 compds.) were prepared. Thus, 2-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me was treated with Me<sub>2</sub>NCH(OMe)<sub>2</sub> to give 2-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>COCH:CHNMe<sub>2</sub>, which was cyclized with NH<sub>2</sub>OH to the isoxazole II (R<sub>4</sub> = NO<sub>2</sub>). Reduction of the nitro group, diazotization, and reaction with SO<sub>2</sub>-HCl gave II (R<sub>4</sub> = SO<sub>2</sub>Cl), which was amidated and treated with BuNCO and COCl<sub>2</sub> to give II (R<sub>4</sub> = SO<sub>2</sub>NCO). Treatment of the isocyanate with 2-amino-4,6-dimethoxypyrimidine gave III which, at 0.05 kg/ha preemergence, gave total control of e.g., nutsedge.

ST benzenesulfonylurea prepn herbicide  
IT Herbicides

(benzenesulfonylureas)

IT 19312-06-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(lithiation and reaction of, with sulfur dioxide)

IT 4205-06-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(methylation of)

IT 87488-64-0P 87488-71-9P 87488-75-3P 87488-81-1P  
87488-85-5P 87488-88-8P 87488-93-5P 87488-96-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and amination of)

IT 87488-99-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and chlorination of)

IT 87488-61-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and cyclization of, with hydroxylamine)

IT 62882-10-4P 87488-63-9P 87488-70-8P 87488-74-2P  
87488-80-0P 87488-92-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and diazotization and reaction of, with sulfur dioxide)

IT 87488-68-4P 87488-73-1P 87488-77-5P 87488-83-3P

87488-87-7P 87488-90-2P 87488-95-7P 87489-01-8P 87489-02-9P

87489-03-0P 87489-04-1P 87489-05-2P 87489-06-3P 87489-07-4P

87489-08-5P 87489-09-6P 87489-10-9P 87489-11-0P

87489-12-1P 87489-13-2P 87489-14-3P 87489-15-4P

87489-16-5P 87489-17-6P 87489-18-7P 87489-19-8P 87489-20-1P

87489-21-2P 87489-22-3P 87489-23-4P 87489-24-5P 87489-25-6P

87489-26-7P 87489-27-8P 87489-28-9P 87489-29-0P 87489-30-3P

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87489-36-9P 87489-37-0P 87489-38-1P 87489-39-2P 87495-41-8P

87495-42-9P 87495-43-0P 87495-44-1P 87495-45-2P

87495-46-3P 87495-47-4P 87495-48-5P 87495-49-6P 87495-50-9P

87495-51-0P 87495-52-1P 87495-53-2P 87495-54-3P 87495-55-4P

87509-99-7P 87510-00-7P 87510-01-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); BIOL (Biological  
study); PREP (Preparation)  
(preparation and herbicidal activity of)

IT 87488-98-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)  
(preparation and methoxylation of)

IT 87488-65-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with Bu isocyanate)

IT 87488-67-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with aminopyrimidine)

IT 87488-97-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with dichlorotriazine isocyanate)

IT 87488-72-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with dimethoxypyrimidinylcarbamate)

IT 87473-90-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with isoxazolylbenzenesulfonamide)

IT 87488-78-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with methylhydrazine)

IT 87488-66-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with phosgene)

IT 87488-82-2P 87488-86-6P 87488-89-9P 87488-94-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with pyrimidinylcarbamate)

IT 87488-76-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with triazinylcarbamate)

IT 37921-17-8P 87488-62-8P 87488-69-5P 87488-79-7P 87488-91-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)

IT 87489-00-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 5234-26-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with DMF dimethylacetal)

IT 83060-43-9 87473-91-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with benzenesulfonamide)

IT 10564-55-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with benzylthiobenzaldehyde)

IT 75-44-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with butylaminocarbonylbenzenesulfonamide)

IT 614-21-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with dimethoxyformamide dimethylacetal)

IT 53868-36-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with hydroxylamine)

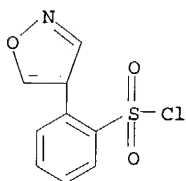
IT 111-36-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with isoxazolylbenzenesulfonamide)

IT 36315-01-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with isoxazolylbenzenesulfonylisocyanate)

IT 4637-24-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with nitroacetophenone)

IT 87488-84-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfur chloride)

IT 24852-71-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with tosylmethyl isocyanide)  
 IT 62882-07-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reduction of)  
 IT 87488-71-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and amination of)  
 RN 87488-71-9 HCAPLUS  
 CN Benzenesulfonyl chloride, 2-(4-isoxazolyl)- (9CI) (CA INDEX NAME)



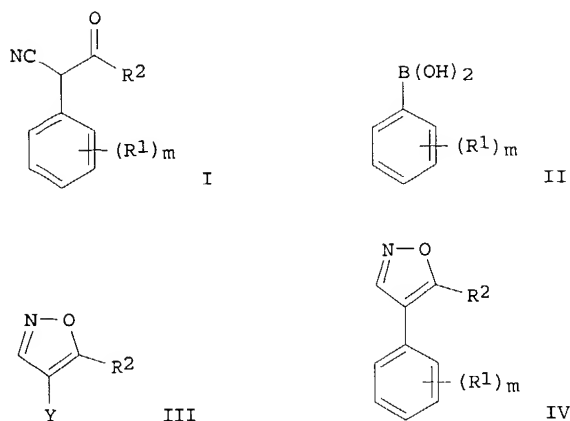
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L28 ANSWER 1 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:368618 HCAPLUS  
 DN 138:368624  
 ED Entered STN: 14 May 2003  
 TI Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic  
 acids and isoxazoles.  
 IN Zhou, Jiacheng; Oh, Lynette May; Ma, Philip  
 PA Bristol-Myers Squibb Pharma Company, USA  
 SO U.S., 20 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D295-033  
 ICS C07D241-04; C07D211-60; C07D207-06; C07C253-12  
 NCL 544059000; 558355000; 558309000; 544159000; 544163000; 544399000;  
 546230000; 548579000  
 CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6562965	B1	20030513	US 2000-610819	20000706
	US 2003208068	A1	20031106	US 2003-387759	20030313 <--
	US 6727360	B2	20040427		
	US 2004171829	A1	20040902	US 2004-786992	20040225 <--
PRAI	US 1998-80680P	P	19980403	<--	
	US 1999-282508	A3	19990331		
	US 2000-610819	A3	20000706		
	US 2003-387759	A3	20030313		

#### CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6562965	ICM	C07D295-033
	ICS	C07D241-04; C07D211-60; C07D207-06; C07C253-12
	NCL	544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000
US 6562965	ECLA	C07C255/41
US 2003208068	ECLA	C07C253/00; C07C255/41; C07D201/08; C07D261/08; C07D261/10B
OS	CASREACT	138:368624; MARPAT 138:368624
GI		



AB .alpha.-Aryl-.beta.-ketonitriles [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], which serve as synthetic intermediates in the preparation of biol. important mols. such as corticotropin releasing factor (CRF) receptor antagonists, were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO<sub>3</sub>, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H<sub>2</sub>O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.

ST arylketonitrile convergent synthesis; nitrile arylketo convergent synthesis

IT Nitriles, preparation

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(oxo; convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 72287-26-4, [1,1'-Bis(diphenylphosphino)ferrocene]palladium dichloride

RL: CAT (Catalyst use); USES (Uses)  
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 246023-57-4P 246023-58-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole

27060-75-9, 4-Bromo-3-methylanisole  
RL: RCT (Reactant); RACT (Reactant or reagent)

(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 7064-37-1P, 4-Bromo-5-Methylisoxazole 7064-38-2P, 4-Iodo-5-methylisoxazole 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P, 4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-methoxybenzeneboronic acid 246023-55-2P 246023-56-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) de Munno, A; J Chem Soc, Perkin Trans 2 1977, 9, P1121 HCAPLUS
- (2) Dominguez, E; J Org Chem 1966, V61, P5435
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- (7) Mitchell, R; J Org Chem 1979, V44, P4733 HCAPLUS
- (8) Olah, G; J Org Chem 1993, V58, P3894

Searched by Noble Jarrell

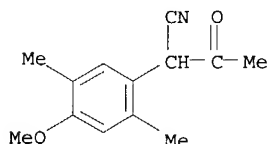
- (9) Olah, G; Journal of Organic Chemistry 1993, V58, P3194 HCAPLUS  
 (10) Rouiller, C; Heterocyclic Compounds-More than One Hetero Atom 1962, P3465  
 (11) Sakakibara, T; Chem Express 1989, V4, P85 HCAPLUS  
 (12) Sumimoto; US 4797492 A 1989 HCAPLUS  
 (13) Zhou; US 6107508 A 2000 HCAPLUS

IT 246023-57-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

RN 246023-57-4 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:965163 HCAPLUS

DN 138:39539

ED Entered STN: 20 Dec 2002

TI Preparation of amino acid derivatives as inhibitors of protein isoprenyl transferases

IN Sebt, Said M.; Hamilton, Andrew D.; Augeri, David J.; Barr, Kenneth J.; Donner, Greg B.; Fakhoury, Stephen A.; O'Connor, Stephen J.; Rosenberg, Saul H.; Shen, Wang; Szczepankiewicz, Bruce G.; Gunawardana, Indrani W.  
 PA University of Pittsburgh, USA

SO U.S. Pat. Appl. Publ., 499 pp., Cont.-in-part of U.S. Ser. No. 852,858, abandoned.

CODEN: USXXCO

DT Patent

LA English

IC ICM C07D045-02

ICS C07D307-56

NCL 544238000; 549321000; 548252000; 544333000; 544405000

CC 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 7, 28, 63

FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002193596	A1	20021219	US 2001-984411	20011030 <--
	US 6693123	B2	20040217		
PRAI	US 1995-7247P	P	19951106	<--	
	US 1996-740909	B2	19961105	<--	
	US 1997-852858	B2	19970507	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2002193596	ICM	C07D045-02
	ICS	C07D307-56
	NCL	544238000; 549321000; 548252000; 544333000; 544405000
US 2002193596	ECLA	C07C237/36; C07D213/70C; C07D213/71; C07D213/71B; C07D213/74E; C07D213/75B2; C07D213/75D3; C07D213/82D; C07D213/82G; C07D213/82H; C07D213/89B; C07D233/54C2D4; C07D233/54C2D2; C07D233/54C2D3; C07D233/54C2D5; C07D233/90; C07D235/06B; C07D237/14; C07D239/26D; C07D239/4B3; C07D241/04; C07D241/12C; C07D241/18; C07D253/06D; C07D257/04D2C1; C07D261/02B; C07D263/2; C07D263/32; C07D265/30C; C07D277/20F1; C07D277/30; C07D277/36; C07D277/48; C07D277/50; C07D295/08B3; C07D295/12B1B1; C07D295/14A3; C07D295/18B1D; C07D295/18B1F; C07D307/54; C07D307/81; C07C239/20; C07D317/30; C07D317/60; C07D333/18; C07D333/20; C07D333/24; C07D401/12; C07D401/12; C07D405/04; C07D405/12; C07D405/12; C07D409/12; C07D417/12; C07D487/08; C07D521/00B1C5; C07D521/00B1N; C07F009/53A7; C07C271/22; C07C317/50; C07C323/59; C07C323/60; C07C327/42; C07D205/04; C07D027/08A; C07D207/09; C07D207/10; C07D207/12; C07D207/26B1;

C07D207/26C; C07D209/48D3A2; C07D021/14; C07D211/42;  
 C07D211/52; C07D211/58; C07D213/30B; C07D213/30C;  
 C07D213/30D2; C07D213/32; C07D213/34; C07D213/36;  
 C07D213/38; C07D213/56; C07D213/64; C07D213/64A;  
 C07D213/65; C07D021/68; C07D213/70B <--

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AB Compds. R3-Z-L1-aryl [aryl is a benzene ring having certain substituents R1, R2, R4; L1 is L4-NR5-L5, L4-O-L5, L4-S(O)m-L5, etc., where L4 and L5 are absent or alk(en)ylene, R5 is H, alkanoyl, alkoxy, alkoxyalkyl, etc.; m = 0-2; Z is a covalent bond, O, S(O)m, an imino group; R3 = (un)substituted pyridyl or imidazolyl; or L1, Z, and R3 together are aminoalkyl, haloalkyl, halo, carboxaldehyde, (carboxaldehyde)alkyl, or hydroxyalkyl (R1 .noteq. H) or L1, Z, R3, and R4 together are an (un)substituted pyrrolidinone ring] were prepared as inhibitors of protein isoprenyl transferases. Thus, N-[4-(3-pyridylcarbonylamino)-2-phenylbenzoyl]methionine hydrochloride, prepared via amidation reaction, showed 93% inhibition of farnesyl transferase at 1x10<sup>-5</sup> M.

ST amino acid deriv prepn inhibitor protein isoprenyl transferase

IT Antiartherosclerotics  
 (antiatherosclerotics; preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT Antitumor agents  
 Atherosclerosis  
 Neoplasm  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT Amino acids, preparation  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT Artery, disease  
 (restenosis; preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 131384-38-8, Protein farnesyltransferase 135371-29-8, Protein geranylgeranyltransferase  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 645-14-7P, 1H-Imidazole-4-acetaldehyde  
 RL: BYP (Byproduct); PREP (Preparation)  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 191100-48-8P 191100-50-2P 191100-75-1P 191101-08-3P 191101-16-3P  
 191101-26-5P 191101-28-7P 191101-51-6P 191101-63-0P 191101-64-1P  
 191102-03-1P 191102-18-8P 478907-80-1P 478908-58-6P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 191100-39-7P 191100-45-5P 191100-74-0P 191100-76-2P 191100-80-8P  
 191100-82-0P 191100-83-1P 191100-84-2P 191100-86-4P 191100-88-6P  
 191100-94-4P 191101-01-6P 191101-04-9P 191101-10-7P 191101-11-8P  
 191101-12-9P 191101-13-0P 191101-14-1P 191101-15-2P 191101-17-4P  
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 191101-35-6P 191101-37-8P 191101-40-3P 191101-42-5P 191101-45-8P  
 191101-47-0P 191101-53-8P 191101-56-1P 191101-58-3P 191101-62-9P  
 191101-65-2P 191101-66-3P 191101-67-4P 191101-68-5P 191101-69-6P  
 191101-71-0P 191101-72-1P 191101-73-2P 191101-74-3P 191101-75-4P  
 191101-76-5P 191101-77-6P 191101-78-7P 191101-80-1P 191101-81-2P  
 191101-82-3P 191101-83-4P 191101-84-5P 191101-85-6P 191101-86-7P  
 191101-88-9P 191101-89-0P 191101-90-3P 191101-91-4P 191101-92-5P  
 191101-93-6P 191101-95-8P 191101-96-9P 191101-97-0P 191101-98-1P  
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 191102-62-2P 191102-63-3P 191102-76-8P 191102-78-0P 191102-79-1DP,  
 1747 191102-79-1P 191102-81-5P 191102-82-6P 191102-83-7P  
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 191105-33-6P 215177-73-4P 215919-73-6P 216229-65-1P 216230-18-1P  
 216232-29-0P 223573-38-4P 225938-38-5P 225938-41-0P 225938-53-4P  
 225938-58-9P 225938-60-3P 225938-64-7P 225938-75-0P 225938-77-2P  
 247235-66-1P 247235-67-2P 247235-68-3P 247235-69-4P 247235-72-9P  
 247235-73-0P 247235-82-1P 251577-09-0P 344900-92-1P 478907-70-9P  
 478907-71-0P 478907-72-1P 478907-73-2P 478907-74-3P 478907-75-4P  
 478907-76-5P 478907-77-6P 478907-78-7P 478907-79-8P 478907-81-2P  
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 478907-93-6P 478907-94-7P 478907-95-8P 478907-96-9P 478907-97-0P  
 478907-98-1P 478907-99-2P 478908-00-8P 478908-01-9P 478908-02-0P  
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 478908-28-0P 478908-29-1P 478908-30-4P 478908-31-5P 478908-32-6P  
 478908-33-7P 478908-34-8P 478908-35-9P 478908-36-0P 478908-37-1P  
 478908-38-2P 478908-39-3P 478908-40-6P 478908-41-7P  
 478908-42-8P 478908-43-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)  
 ; USES (Uses)

(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 478908-44-0P 478908-45-1P 478908-46-2P 478908-47-3P 478908-48-4P  
 478908-49-5P 478908-50-8P 478908-51-9P 478908-52-0P 478908-53-1P  
 478908-54-2P 478908-55-3P 478908-56-4P 478908-57-5P 478908-59-7P  
 478908-60-0P 478908-61-1P 478908-62-2P 478909-39-6P 478909-40-9P  
 478909-41-0P 478909-42-1P 478909-43-2P 478909-44-3P 478909-45-4P  
 478909-46-5P 478909-47-6P 478909-48-7P 478909-49-8P 478909-50-1P  
 478909-51-2P 478909-52-3P 478909-53-4P 478909-54-5P 478909-55-6P  
 478909-73-8P 478909-74-9P 478909-75-0P 478909-76-1P 478909-77-2P  
 478909-78-3P 478909-79-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 59-67-6, Nicotinic acid, reactions 61-90-5, L-Leucine, reactions  
 85-46-1, 1-Naphthalenesulfonyl chloride 93-11-8, 2-Naphthalenesulfonyl  
 chloride 96-26-4, 1,3 Dihydroxyacetone 98-10-2, Benzenesulfonamide  
 98-58-8 98-59-9 98-60-2 98-68-0 98-74-8 98-80-6, Phenylboronic  
 acid 100-55-0, 3-Pyridinemethanol 106-93-4, 1 2 Dibromoethane  
 108-95-2, Phenol, reactions 109-00-2, 3 Hydroxypyridine 123-62-6,  
 Propionic anhydride 133-59-5, Benzenesulfonyl chloride, 2 methyl  
 150-13-0, 4 Aminobenzoic acid 288-32-4, Imidazole, reactions 327-57-1,  
 L-Norleucine 349-88-2 372-39-4, 3 5 Difluoroaniline 462-08-8, 3  
 Aminopyridine 500-22-1, 3 Pyridinecarboxaldehyde 504-24-5, 4  
 Aminopyridine 504-29-0, 2 Aminopyridine 513-35-9, 2 Methyl 2 butene  
 536-74-3, Phenylacetylene 556-96-7, 5 Bromo m xylene 590-97-6,  
 Bromomethyl acetate 591-22-0, 3 5 Dimethylpyridine 594-44-5,  
 Ethylsulfonyl chloride 626-61-9 700-38-9, 3 Hydroxy 4 nitrotoluene  
 777-44-6 872-85-5, 4-Pyridinecarboxaldehyde 917-92-0,  
 tert-Butylacetylene 934-56-5 994-89-8, Ethynyltributyltin 1072-63-5,  
 1-Vinylimidazole 1120-87-2, 4 Bromopyridine 1122-58-3, 4  
 Dimethylaminopyridine 1739-84-0, 1 2 Dimethylimidazole 1899-93-0  
 1939-99-7, Benzylsulfonyl chloride 2185-02-6, L-Homoserine lactone  
 2208-07-3, Ethyl acetimidate hydrochloride 2315-36-8, 2 Chloro n n  
 diethylacetamide 2486-69-3, 4 Amino 3 methoxybenzoic acid 2486-70-6, 4  
 Amino 3 methylbenzoic acid 2488-15-5 2491-18-1, L Methionine methyl  
 ester hydrochloride 2537-48-6, Diethyl cyanomethylphosphonate  
 2666-93-5, L-Leucine methyl ester 2991-42-6 3081-61-6 3081-62-7  
 3251-69-2, 4 Imidazoleacetic acid hydrochloride 3844-54-0 3900-89-8  
 4670-56-8 5036-48-6, 1H-Imidazole-1-propanamine 5292-45-5 5337-09-7  
 5372-81-6 5446-02-6 5720-05-8, 4 Methylphenylboronic acid 5720-06-9,  
 2 Methoxyphenylboronic acid 5720-07-0, 4 Methoxyphenylboronic acid  
 5832-44-0 6224-91-5, 1 Trimethylsilyl 1 propyne 6959-48-4, 3  
 Chloromethylpyridine hydrochloride 7745-93-9, 2 Bromo 4 nitrotoluene  
 10065-72-2, L-Alanine methyl ester 10111-08-7, 2 Imidazolecarboxaldehyde  
 10147-37-2, Isopropylsulfonyl chloride 10365-98-7, 3  
 Methoxyphenylboronic acid 13324-11-3 13922-41-3, 1 Naphthaleneboronic

acid 15084-51-2 15399-22-1 16419-60-6, 2-Methylphenylboronic acid  
 16420-13-6, Dimethylthiocarbamoyl chloride 16712-69-9 17933-03-8, 3  
 Methylphenylboronic acid 18997-19-8, Chloromethyl pivalate 20260-53-1,  
 Nicotinic acid chloride hydrochloride 22840-14-8 25999-04-6,  
 4-Morpholinesulfonamide 27784-76-5, tert-Butyl diethylphosphonoacetate  
 29604-19-1 29681-44-5 30925-18-9 31872-62-5, 4-Methoxy 3  
 nitropyridine 32085-88-4, 3 5 Difluorobenzaldehyde 32673-41-9, 4  
 Hydroxymethylimidazole hydrochloride 35454-39-8 39555-28-7,  
 2-Adamantaneethanol 51175-71-4, 3-Thiophenesulfonyl chloride  
 52536-09-1 53317-09-2 58728-64-6, 4 Amino 1 naphthalenecarbonitrile  
 67492-50-6 67753-90-6 68559-40-0 74763-88-5 79538-20-8, 3 5  
 Difluorobenzyl alcohol 90002-36-1 100959-22-6 114081-08-2  
 136789-15-6 152620-34-3 158063-66-2 165534-79-2 166169-26-2  
 180977-33-7 191105-36-9 191105-39-2 191105-40-5 191105-41-6  
 191105-43-8 191105-44-9 191105-46-1 215177-71-2 215919-24-7  
 302964-21-2 318290-86-7 345964-93-4 478909-57-8 478909-59-0  
 478909-61-4 478909-62-5 478909-63-6 478909-64-7 478909-67-0  
 478909-68-1 478909-72-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl  
 transferases)

IT 1121-55-7P, 3 Vinylpyridine 2150-47-2P 3430-27-1P 7314-32-1P  
 13480-38-1P, 4 Nitro 2 phenyltoluene 13511-89-2P 15144-85-1P  
 16426-64-5P, 2 Bromo 4 nitro benzoic acid 25539-19-9P 31434-93-2P  
 32018-87-4P, 4 Amino 1 naphthoic acid 33016-47-6P 33769-07-2P  
 34805-23-7P 38940-67-9P 45533-87-7P, 4 Hydroxymethyl 2 methylimidazole  
 51990-95-5P 62199-60-4P 66493-39-8P 80715-22-6P 84269-70-5P  
 84539-35-5P 85391-05-5P 88181-49-1P 92254-03-0P 102676-60-8P  
 105183-60-6P 106945-71-5P 114077-82-6P 117504-12-8P 118054-54-9P  
 124391-60-2P, 4 Nitro 2 phenylbenzoic acid 131249-78-0P 133728-31-1P  
 149543-83-9P 160446-35-5P 160813-66-1P 164362-16-7P 166169-27-3P  
 166170-19-0P 168169-12-8P 172975-69-8P, 3 5 Dimethylphenylboronic acid  
 173472-36-1P 179015-63-5P 180863-46-1P 180863-47-2P 180863-61-0P  
 180976-91-4P 180976-94-7P 180976-95-8P 180976-96-9P 180976-98-1P  
 180976-99-2P 180977-00-8P 180977-02-0P 180977-03-1P 180977-05-3P  
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 182499-91-8P 182500-28-3P 185051-42-7P 191101-18-5P 191101-20-9P  
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 191103-72-7P 191103-73-8P 191103-74-9P 191103-75-0P 191103-76-1P  
 191103-77-2P 191103-78-3P 191103-80-7P 191103-85-2P 191103-86-3P  
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 191104-94-6P 191104-95-7P 191104-96-8P 191104-97-9P 191104-98-0P  
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 478908-79-1P 478908-80-4P 478908-81-5P 478908-82-6P 478908-83-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of amino acid derivs. as inhibitors of protein isoprenyl  
 transferases)

IT 478908-84-8P 478908-85-9P 478908-86-0P 478908-87-1P 478908-88-2P



478908-89-3P 478908-90-6P 478908-91-7P 478908-92-8P 478908-93-9P  
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 478909-56-7P 478909-58-9P 478909-60-3P 478909-65-8P 478909-66-9P  
 478909-69-2P 478909-70-5P 478909-71-6P 478909-80-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of amino acid derivs. as inhibitors of protein isoprenyl  
 transferases)

IT 478908-40-6P

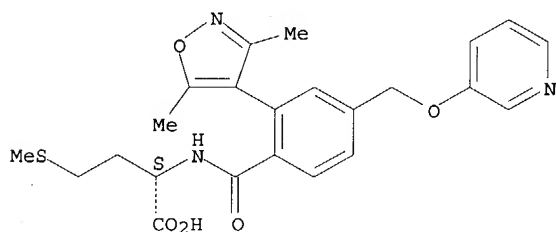
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)  
 ; USES (Uses)

(preparation of amino acid derivs. as inhibitors of protein isoprenyl  
 transferases)

RN 478908-40-6 HCAPLUS

CN L-Methionine, N-[2-(3,5-dimethyl-4-isoxazolyl)-4-[(3-  
 pyridinyloxy)methyl]benzoyl]-, monolithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Li

L28 ANSWER 3 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:369024 HCAPLUS

DN 136:369710

ED Entered STN: 18 May 2002

TI Preparation of heterocyclo substituted hydroxamic acid derivatives as  
 cyclooxygenase-2 and 5-lipoxygenase inhibitors

IN Talley, John J.; Sikorski, James A.; Graneto, Matthew J.; Carter, Jeffery  
 S.; Norman, Bryan H.; Devadas, Balekudru

PA Pharmacia Corp., USA

SO U.S. Pat. Appl. Publ., 54 pp., Cont. of U. S. Ser. No. 624,301.

CODEN: USXXCO

DT Patent

LA English

IC ICM C07D043-04

NCL 544238000

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

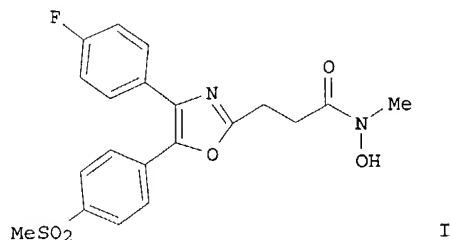
FAN.CNT 1

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PI	US 2002058810	A1	20020516	US 2001-997633	20011129 <--
	US 6696477	B2	20040224		
PRAI	US 1995-450545	A1	19950717	<--	
	US 1997-822528	B1	19970324	<--	
	US 1998-218921	B1	19981222	<--	
	US 2000-624301	A1	20000724		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2002058810	ICM	C07D043-04
	NCL	544238000

US 2002058810 ECLA B60G017/015C; B64C027/00B; F16F007/10A; F16F015/03 <--  
 OS MARPAT 136:369710  
 GI



- AB Compds. of the formula R2SO2-4-C6H4-A(R1)YR3NR4R5 [A = 5 or 6 membered heterocyclic or carbocyclic ring; Y = alkyl, alkynyl, alkenyl, aryl, aralkyl, cycloalkyl; R1 = heterocyclyl, cycloalkyl, aryl, cycloalkenyl; R2 = alkyl, amino; R3 = bond, CO, (substituted) NHCO, S-CS; R4 = H, OH, alkyl, aryl heterocyclyl, cycloalkyl; R5 = H, alkyl, aryl, heterocyclyl, cycloalkyl] are prepared as antiinflammatory agents. The compds. are useful for treating disorders mediated by cyclooxygenase-2 or 5-lipoxygenase, such as inflammation. Thus, I was prepared from 4-(4-fluorophenyl)-5-(4-(methylsulfonyl)phenyl)-2-oxazolepropionic acid. The IC50 of I was 5.2 .mu.M for COX-2 and 0.05 .mu.M for 5-LO.
- ST heterocyclo hydroxamic acid deriv prepn cyclooxygenase inhibitor;  
 lipoxygenase heterocyclo hydroxamic acid deriv prepn inhibitor;  
 antiinflammatory heterocyclo hydroxamic acid deriv prepn
- IT Allergy inhibitors  
 Analgesics  
 Anti-inflammatory agents  
 Antiarthritics  
 Antiasthmatics  
 (preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)
- IT Hydroxamic acids  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)
- IT Fever and Hyperthermia  
 (treatment; preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)
- IT 80619-02-9, 5-Lipoxygenase 329900-75-6, Cyclooxygenase-2 329967-85-3, Cyclooxygenase-1  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (inhibitors; preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)
- IT 185826-83-9P 185826-85-1P 185826-87-3P 425417-15-8P 425417-17-0P  
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 425417-27-2P 425417-29-4P 425417-30-7P 425417-33-0P 425417-35-2P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)  
 ; USES (Uses)

(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and  
 5-lipoxygenase inhibitors)

IT 99-91-2 553-90-2, Dimethyl oxalate 17852-52-7 163303-39-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and  
 5-lipoxygenase inhibitors)

IT 39757-35-2P 170570-50-0P 170571-19-4P 170571-20-7P 170571-48-9P

170571-71-8P 185826-92-0P 185826-97-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and  
 5-lipoxygenase inhibitors)

IT 425417-77-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

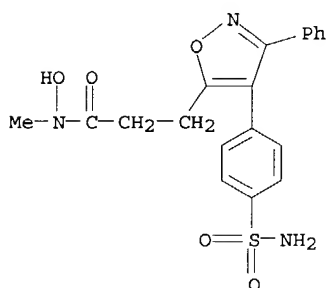
THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)

; USES (Uses)

(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and  
 5-lipoxygenase inhibitors)

RN 425417-77-2 HCAPLUS

CN 5-isoxazolepropanamide, 4-[4-(aminosulfonyl)phenyl]-N-hydroxy-N-methyl-3-  
 phenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 4 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:84600 HCAPLUS

DN 136:151161

ED Entered STN: 31 Jan 2002

TI Preparation of 4-(heterocyclyl)benzenesulfonamides as components of a  
 combination of a cyclooxygenase-2 inhibitors and a leukotriene B4 receptor  
 antagonist

IN Isakson, Peter C.; Anderson, Gary D.; Gregory, Susan A.

PA G.D. Searle and Co., USA

SO U.S., 19 pp., Cont.-in-part of U.S. Ser. No. 489,415, abandoned.

CODEN: USXXAM

DT Patent

LA English

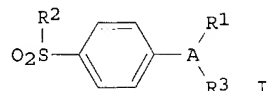
IC ICM A61K031-415  
ICS C07D231-02; C07D231-12  
NCL 514326000  
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6342510	B1	20020129	US 1996-661641	19960611 <--
	CA 2224563	AA	19961227	CA 1996-2224563	19960611 <--
	US 2002107276	A1	20020808	US 2002-38080	20020103 <--
PRAI	US 1995-489415	B2	19950612	<--	
	US 1996-661641	A1	19960611	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6342510	ICM	A61K031-415
	ICS	C07D231-02; C07D231-12
	NCL	514326000
US 2002107276	ECLA	A61K045/06 <--
OS	MARPAT 136:151161	
GI		



AB The title compds. [I; A = (partially) unsatd. heterocyclyl or carbocyclyl; R1 = (un)substituted heterocyclyl, cycloalkyl, cycloalkenyl, aryl; R2 = Me, NH2; R3 = H, halo, alkyl, etc.] which are cyclooxygenase-2 inhibitors used in combination with a leukotriene B4 receptor antagonists for treatment of inflammation and inflammation-related disorders, were prepared and formulated. Thus, treating Et trifluoroacetate with NaOMe in Me tert-Bu ether followed by addition of 4'-chloroacetophenone (85%), and reacting the resulting 4,4,4 trifluoro-1-(4-chlorophenyl)butane 1,3 dione with 4-sulfonamidophenylhydrazine hydrochloride in EtOH afforded 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (80%).

ST heterocyclylbenzenesulfonamide prepn cyclooxygenase COX2 inhibitor combination leukotriene B4; antiarthritic heterocyclylbenzenesulfonamide prepn; antiinflammatory heterocyclylbenzenesulfonamide prepn

IT Leukotriene receptors  
RL: BSU (Biological study, unclassified); BIOL (Biological study) (leukotriene B4; preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT Anti-inflammatory agents  
Antiarthritics (preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 329900-75-6, Cyclooxygenase-2  
RL: BSU (Biological study, unclassified); BIOL (Biological study) (preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 93014-16-5P, 4-[2-Methyl-4-phenyl-5-oxazolyl]benzenesulfonamide 169590-41-4P, 4-[5-(3-Fluoro-4-methoxyphenyl)-3-(difluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 169590-42-5P, 4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 170569-86-5P, 4-[5-(4-Chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 177660-80-9P, 2-Methyl-5-[1-[4-(methylsulfonyl)phenyl]-4-trifluoromethyl-1H-imidazol-2-yl]pyridine 177660-92-3P, 4-[2-(5-Methylpyridin-3-yl)-4-(trifluoromethyl)-1H-imidazol-1-yl]benzenesulfonamide 181695-72-7P, 4-[5-Methyl-3-phenylisoxazol-4-yl]benzenesulfonamide 185344-51-8P, 4-[2-Trifluoromethyl-5-(3,4-difluorophenyl)-4-oxazolyl]benzenesulfonamide 185344-55-2P, 4-[2-Trifluoromethyl-5-(3-fluoro-4-methoxyphenyl)-4-oxazolyl]benzenesulfonamide 195061-34-8P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 99-91-2, 4'-Chloroacetophenone 321-28-8, 2-Fluoroanisole 383-63-1,

Ethyl trifluoroacetate 454-31-9, Ethyl difluoroacetate 27918-19-0,  
4-Sulfonamidophenylhydrazine hydrochloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as  
antiinflammatories)

IT 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 18931-60-7P,  
4,4,4-Trifluoro-1-[4-chlorophenyl]butane-1,3-dione 170570-77-1P,  
4,4-Difluoro-1-(3-fluoro-4-methoxyphenyl)butane-1,3-dione  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as  
antiinflammatories)

IT 60940-34-3, Ebselen 71125-38-7, Meloxicam 80937-31-1, Flosulide  
110501-66-1, TMK 688 117423-95-7, LY 213024 123653-11-2, Taisho NS 398  
128253-31-6, Bay-X 1005 133430-69-0, ETH 615 134578-96-4, ONO 4057  
135199-82-5, LY 264086 135893-33-3, PF 10042 136326-31-3, WAY 121006  
142422-79-5, RP 66153 146461-98-5, SM 15178 147398-01-4, CGS 25019C  
147432-77-7, BI RM 270 150399-22-7, SB 201993 153633-01-3, SC 53228  
161172-51-6, LY 293111 162011-90-7, 2(5H)-Furanone, 4-[4-  
(methylsulfonyl)phenyl]-3-phenyl- 180208-37-1, SB 201146  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as  
antiinflammatories)

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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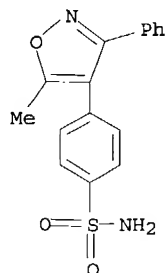
- (1) Anon; EP 485111 1992 HCAPLUS
  - (2) Anon; WO 9404522 1994 HCAPLUS
  - (3) Anon; WO 9413635 1994 HCAPLUS
  - (4) Anon; WO 9415932 1994 HCAPLUS
  - (5) Anon; WO 9420480 1994 HCAPLUS
  - (6) Anon; WO 9426731 1994 HCAPLUS
  - (7) Anon; WO 9427980 1994 HCAPLUS
  - (8) Anon; WO 9500501 1994 HCAPLUS
  - (9) Anon; DE A4228201 1994
  - (10) Anon; WO 9603387 1996 HCAPLUS
  - (11) Anon; WO 9603388 1996 HCAPLUS
  - (12) Anon; WO 9606840 1996 HCAPLUS
  - (13) Anon; J Allergy Clinl Immunol 1988, V81, P110
  - (14) Anon; J Basamajian Spine 1989, V14, P438
  - (15) Beaver; Am J Med 1984, V77, P38 HCAPLUS
  - (16) Chang; Acta Pharmacologica Sinica 1991, V12(2), P121 HCAPLUS
  - (17) Deason; US 4923891 A 1990 HCAPLUS
  - (18) Dereu; US 5366982 A 1994 HCAPLUS
  - (19) Djuric; US 4970234 A 1990 HCAPLUS
  - (20) Djuric; US 5212198 A 1993 HCAPLUS
  - (21) Djuric; US 5310951 A 1994 HCAPLUS
  - (22) Djuric; US 5380740 A 1995 HCAPLUS
  - (23) Ducharme; US 5474995 A 1995 HCAPLUS
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  - (29) Huang; US 5210208 A 1993 HCAPLUS
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  - (32) Isakson; US 5700816 A 1997 HCAPLUS
  - (33) Konno; US 5256686 A 1993 HCAPLUS
  - (34) Lau; US 5510368 A 1996 HCAPLUS
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  - (36) Main; US 5246965 A 1993 HCAPLUS
  - (37) Mueller; US 5272178 A 1993 HCAPLUS
  - (38) Musser; US 4889935 A 1989 HCAPLUS
  - (39) Norman; US 5380738 A 1995 HCAPLUS
  - (40) Reitz; US 5344991 A 1994 HCAPLUS
  - (41) Reitz; US 5393790 A 1995 HCAPLUS
  - (42) Seideman; Acta Orthop Scand 1993, V64, P285 MEDLINE
  - (43) Seifert; Curr Med Res Opin 1980, V7, P38 MEDLINE
  - (44) Stewart; Clin Pharmacol Ther 1990, V47, P540 MEDLINE
  - (45) Talley; US 5434178 A 1995 HCAPLUS
  - (46) Talley; US 5466823 A 1995 HCAPLUS
  - (47) Teicher; Cancer Chemother Pharmacol 1994, V33, P515 HCAPLUS
  - (48) Tennant; J Pharm Pharmacol 1987, V39, P309 HCAPLUS
  - (49) Trampusch; Inflammation 1993, V17, P531 HCAPLUS
  - (50) Willikens; Arthritis Rheum 1976, V19, P677
- IT 181695-72-7P, 4-[5-Methyl-3-phenylisoxazol-4-yl]benzenesulfonamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)  
; USES (Uses)

(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as  
antiinflammatories)

RN 181695-72-7 HCAPLUS

CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX  
NAME)



L28 ANSWER 5 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:813420 HCAPLUS

DN 135:344507

ED Entered STN: 08 Nov 2001

TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing  
factor (CRF) antagonists

IN He, Ligi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios

PA Dupont Pharmaceuticals Company, USA

SO U.S., 57 pp., Cont.-in-part of U.S. Ser. No. 899,242.

CODEN: USXXAM

DT Patent

LA English

IC A61K031-535; C07D487-04

NCL 514246000

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 2, 63

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6313124	B1	20011106	US 1998-14734	19980128 <--
	US 6124289	A	20000926	US 1997-899242	19970723 <--
	ZA 9706603	A	19990125	ZA 1997-6603	19970724 <--
	US 6136809	A	20001024	US 1998-14999	19980128 <--
	LT 4680	B	20000725	LT 1999-8	19990125 <--
	CA 2314613	AA	19990805	CA 1999-2314613	19990128 <--
	WO 9938868	A1	19990805	WO 1999-US1824	19990128 <--
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,				
	PT, SE				
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	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128 <--
	EP 1049699	B1	20040421		
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	SI, LT, LV, FI, RO				
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	EP 1344779	A1	20030917	EP 2003-75887	19990128 <--
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	TW 520372	B	20030211	TW 1999-88102636	19990223 <--
	US 2003008885	A1	20030109	US 2001-930782	20010816 <--
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	US 1997-899242	A2	19970723	<--	
	US 1998-14734	A	19980128	<--	
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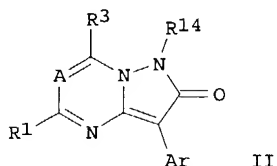
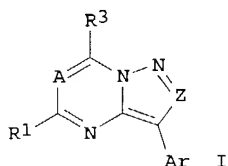
WO 1999-US1824

W

19990128

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6313124	IC	A61K031-535IC C07D487-04
	NCL	514246000
EP 1344779	ECLA	C07D487/04; C07D487/04 <--
US 2003008885	ECLA	C07D487/04; C07D487/04; C07D487/04 <--
OS MARPAT 135:344507		
GI		



- AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists (no data) which are useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl) [1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline, followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dichlorophenyl) [1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxy-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].
- ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor antagonist azolotriazine azolopyrimidine prepn
- IT Corticotropin releasing factor receptors  
 RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)
- IT 202578-49-2P 202579-55-3P 202579-56-4P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 105-53-3, Diethyl malonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1000-84-6 1445-45-0, Trimethyl orthoacetate 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetone nitrile 78531-29-0 202580-72-1 202580-73-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one 202580-62-9P, 5-Amino-4-(2,4-dimethylphenyl)-3-methylpyrazole 202580-64-1P 202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P  
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 (preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

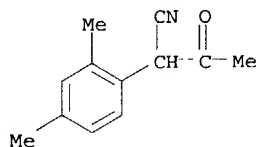
RE.CNT 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD

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 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)  
 RN 202580-61-8 HCAPLUS  
 CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



DN 134:178572  
 ED Entered STN: 22 Feb 2001  
 TI Preparation of azolo triazines and pyrimidines as corticotropin releasing factor (CRF) antagonists  
 IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios  
 PA Dupont Pharmaceuticals Co., USA  
 SO U.S., 90 pp., Cont.-in-part of U. S. Ser. No. 899,242.  
 CODEN: USXXAM

DT Patent

LA English

IC ICM C07D487-04

ICS C07D251-72; A61K031-53

NCL 514246000

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

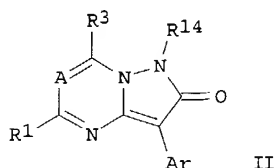
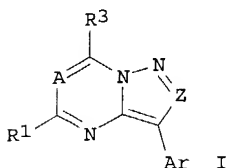
Section cross-reference(s): 1, 2, 63

FAN.CNT 5

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	US 6136809	A	20001024	US 1998-14999	19980128 <--
	LT 4680	B	20000725	LT 1999-8	19990125 <--
	CA 2314613	AA	19990805	CA 1999-2314613	19990128 <--
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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	ICS	C07D251-72; A61K031-53
	NCL	514246000
EP 1344779	ECLA	C07D487/04; C07D487/04
OS	MARPAT	134:178572
GI		



AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alk(en/yn)yl, halo, etc.; R1, R2 = H, alk(en/yn)yl, halo, etc.; R3 = H, SH, aryl, etc.; R14 = (un)substituted alk(en/yn)yl, cycloalkyl(alkyl)], useful in treating CRF-related

disorders, particularly anxiety, depression, and other psychiatric, neurol. disorders as well as treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. For instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-2,5-dimethyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl<sub>3</sub> and PhNET<sub>2</sub> to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound I [A = CH; R<sub>1</sub> = Me; R<sub>3</sub> = NHCHET<sub>2</sub>; Z = CMe; Ar = 2-Cl-4-MeC<sub>6</sub>H<sub>3</sub>]. The compds. I are effective at 0.002-200 mg/kg/day.

ST azolo triazine pyrimidine prepn formulation CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine prepn formulation CRF receptor antagonist; azolopyrimidine prepn formulation CRF receptor antagonist  
IT Antidepressants  
Anxiolytics

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)  
IT Corticotropin releasing factor receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)  
IT 202578-49-2P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT	105-53-3, Diethyl malonate	105-58-8, Diethyl carbonate	141-97-9, Ethyl acetoacetate
	616-24-0, 3-Pentylamine	622-79-7, Benzyl azide	
	1445-45-0, Trimethyl orthoacetate	2208-07-3	34688-71-6,

2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile

78531-29-0 202580-72-1 202580-73-2 326821-97-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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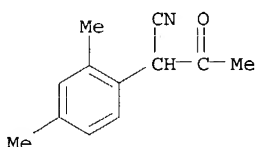
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- IT 202580-61-8P

(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RN 202580-61-8 HCAPLUS

CN Benzeneacetone nitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



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L28 ANSWER 7 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:307132 HCAPLUS
DN 132:321873
ED Entered STN: 12 May 2000
TI Azolo triazines and pyrimidines useful as corticotropin releasing factor
(CRF) antagonists
IN Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA DuPont Pharmaceuticals Co., USA
SO U.S., 86 pp., Cont.-in-part of U.S. Ser. No. 899,242.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-505
ICS C07D487-04
NCL 514258000
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2
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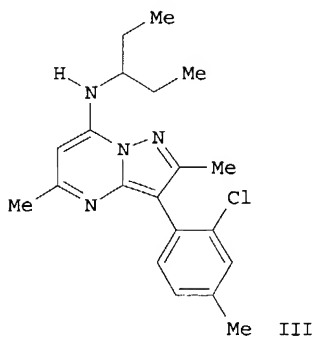
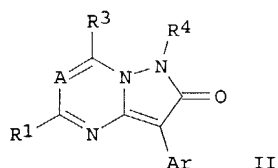
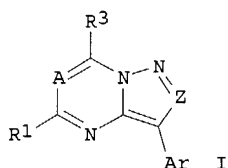
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	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,				

PT, SE

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AU 748818	B2	20020613		
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## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6060478	ICM	A61K031-505	
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	NCL	514258000	
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EP 1344779	ECLA	C07D487/04; C07D487/04	<--
OS MARPAT 132:321873			
GI			



AB Corticotropin releasing factor (CRF) antagonists (no data) of formulas I and II are disclosed [wherein A = N or CR; Z = N or CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, pyrimidinyl, indanyl, tetralinyl, addnl. selected heterocycles; R = H, alk(en/yn)yl, cycloalkyl(alkyl), halo, cyano, haloalkyl; R1, R2 = H, groups listed for R, NH2 or derivs., OH or derivs., SH or derivs., addnl. substituted alkyls; R3 = H, OH or derivs., SH or derivs., acyl, CO2H or esters, NH2 or derivs., aryl, heteroaryl, alk(en/yn)yl, etc.; R4 = (un)substituted alk(en/yn)yl or cycloalkyl(alkyl)]. The compds. are of use in the treatment of CRF-related disorders, particularly anxiety and depression, as well as other psychiatric, neurol., immunol., cardiovascular, and psychopathol. disorders. For instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-

methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-5-methyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl<sub>3</sub> and PhNET<sub>2</sub> to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound III.

- ST azolo triazine pyrimidine prepn CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine azolopyrimidine prepn CRF receptor antagonist
- IT Drugs  
(gastrointestinal; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT Intestine, disease  
(irritable bowel syndrome, treatment; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT Anti-inflammatory agents  
Antidepressants  
Anxiolytics  
Cardiovascular agents  
Immunomodulators  
Nervous system agents  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT Corticotropin releasing factor receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT 1000-84-6P 202578-49-2P 202578-50-5P 202579-55-3P 202579-56-4P  
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202580-62-9P 202580-64-1P 202580-66-3P 202580-68-5P 202580-69-6P  
202580-70-9P 234778-65-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT 9015-71-8, Corticotropin releasing factor  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT 105-53-3, Diethyl malonate 105-58-8 141-78-6, Acetic acid ethyl ester, reactions 141-97-9 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1445-45-0, Trimethyl orthoacetate 2208-07-3 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile 78531-29-0, 1,3-Dimethoxy-2-aminopropane 202580-72-1 202580-73-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(starting material; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
- IT 202578-52-7P 202578-53-8P 202578-54-9P 202578-55-0P 202578-57-2P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

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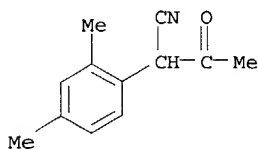
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD

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 IT 202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of azolo-fused triazines and pyrimidines as CRF  
 antagonists)  
 RN 202580-61-8 HCAPLUS  
 CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 8 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:152295 HCAPLUS  
 DN 130:209711  
 ED Entered STN: 09 Mar 1999  
 TI Preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor  
 antagonists  
 IN Caldwell, Charles G.; Chiang, Yuan-ching; Dorn, Conrad; Finke, Paul; Hale,  
 Jeffrey; Maccoss, Malcolm; Mills, Sander; Robichaud, Albert  
 PA Merck and Co., Inc., USA  
 SO U.S., 98 pp.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC ICM A61K031-36  
 ICS C07D285-04; C07D307-94; C07D311-96  
 NCL 514337000  
 CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5877191	A	19990302	US 1997-955898	19971022 <--
PRAI US 1997-955898		19971022 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5877191	ICM	A61K031-36
	ICS	C07D285-04; C07D307-94; C07D311-96
	NCL	514337000

OS MARPAT 130:209711  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention is directed to certain novel compds. represented by structural formula [I; R3 is selected from hydrogen, C1-8 alkyl, R4, R4-substituted C1-6 alkyl; R4 is hydroxy, C1-6 alkoxy, phenyl-C1-3 alkoxy, Ph, cyano, halo, (un)substituted NH2, heterocyclyl, (un)substituted CO2H, etc.; R6, R7, and R8 are selected from hydrogen, C1-6 alkyl, halo, (un)substituted C1-6 alkyl, HO, cyano, CF3, CF3O, OCF2H, OCFH2, NO2, SH, C1-6 alkylthio, (un)substituted CO2H or NH2, heterocyclyl, C1-6 alkylheterocyclyl, etc.; R11, R12, and R13 are selected from hydrogen, (un)substituted C1-6 alkyl, halo, cyano, CF3, NO2, HO, C1-6 alkoxy, acyl, (un)substituted CO2H or NH2, etc.; m is an integer of 1 or 2; n is an integer of 0, 1, or 2]. A method for antagonizing the effect of substance P at its receptor site or for the blockade of neurokinin-1 receptors in a mammal comprises the administration to the mammal of the above compound in an amount that is effective for antagonizing the effect of substance P at its receptor site or for the blockade of neurokinin-1 receptors in the mammal. The invention is also concerned with pharmaceutical formulations comprising these novel compds. as active ingredients and the use of the novel compds. and their formulations in the treatment of certain disorders. The compds. of this invention are useful in the treatment of inflammatory diseases, pain or migraine, asthma, and emesis (no data). Thus, Me [5(RS),6(SR),7(SR)]-6-(4-fluorophenyl)-3-(trimethylstannyl)-1-oxaspiro[4,4]non-3-ene-7-carboxylate was coupled with 3-bromo-4-(5-(trifluoromethyl)tetrazol-1-yl)anisole in the presence of tetrakis(triphenylphosphine)palladium(0) in dioxane at 100.degree. for 1.5 h to give the title compound, Me 5-((5-(trifluoromethyl)tetrazol-1-yl)phenyl)-1-oxaspiro[4.4]nonane-7-carboxylate derivative (II).

ST phenyl spiro cycloalkyl ether prepn tachykinin receptor antagonist; substance P receptor antagonist; neurokinin 1 receptor blocker; inflammatory disease treatment oxaspiro[4.4]nonane; pain treatment oxaspiro[4.4]nonane; migraine treatment oxaspiro[4.4]nonane; asthma treatment oxaspiro[4.4]nonane; emesis treatment oxaspiro[4.4]nonane; tetrazolylphenyloxaspiro[4.4]nonane prepn tachykinin receptor antagonist; oxaspiro[4.4]nonane tetrazolyl phenyl prepn tachykinin receptor antagonist

IT Tachykinin receptors  
 (NK1 antagonists; preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT Tachykinin receptors  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (antagonists; preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT Headache  
 (migraine; preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT Analgesics  
 Antiasthmatics  
 Antiemetics  
 (preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT 33507-63-0, Substance P

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT 50-00-0, Formaldehyde, reactions 57-14-7, 1,1-Dimethylhydrazine  
74-88-4, Iodomethane, reactions 75-16-1, Methylmagnesium bromide  
75-30-9, 2-Iodopropane 79-24-3, Nitroethane 99-89-8, 4-Isopropylphenol  
100-51-6, Benzyl alcohol, reactions 100-52-7, Benzaldehyde, reactions  
103-71-9, Phenyl isocyanate, reactions 105-56-6, Ethyl cyanoacetate  
108-24-7 110-13-4, 2,5-Hexanedione 110-91-8, Morpholine, reactions  
123-75-1, Pyrrolidine, reactions 328-93-8, 2,5-Bis-  
trifluoromethylaniline 334-88-3, Diazomethane 402-10-8,  
2-Bromo-4-(trifluoromethyl)anisole 407-25-0, Trifluoroacetic anhydride  
459-57-4, 4-Fluorobenzaldehyde 460-08-2, 2-Fluoroethylamine  
hydrochloride 623-71-2, Ethyl .beta.-chloropropionate 645-36-3,  
Aminoacetaldehyde diethyl acetal 661-69-8, Hexamethylditin 828-27-3,  
4-Trifluoromethoxyphenol 1427-07-2, 3-Fluoro-4-methylnitrobenzene  
1515-78-2, 1-Phenyl-1,3-butadiene 1544-85-0, 2,2-Difluoro-5-  
aminobenzodioxole 2627-86-3, (S)-(-)-.alpha.-Methylbenzyl amine  
2967-66-0, Methyl 4-(trifluoromethyl)benzoate 3886-69-9,  
(R)-.alpha.-Methylbenzyl amine 4009-98-7, (Methoxymethyl)triphenylphosph  
onium chloride 5197-28-4, 2-Bromo-4-nitroanisole 5470-11-1,  
Hydroxylamine hydrochloride 6423-74-1, 3-Bromo-4-isopropoxybenzonitrile  
7051-34-5, Bromomethylcyclopropane 7143-01-3, Methanesulfonic anhydride  
13296-94-1, 2-Bromo-4-nitroaniline 16911-89-0, Phenyl  
chlorodithioformate 18962-05-5, 4-Isopropoxybenzaldehyde 24424-99-5,  
Di-tert-butyl dicarbonate 26386-88-9, Diphenylphosphoryl azide  
34841-06-0, 3-Bromo-4-methoxybenzaldehyde 44637-25-4,  
Trifluoroacetylhydroxymoyl bromide 69739-34-0, tert-Butyldimethylsilyl  
triflate 80522-42-5, Triisopropylsilyl triflate 81107-97-3,  
2-Bromo-4-(trifluoromethyl)phenol 99583-51-4, 3-Acetoxy-2-  
[(trimethylstannyl)methyl]-1-propene 145100-51-2 191602-55-8  
200956-54-3, 2-Bromo-1-isopropoxy-4-(trifluoromethyl)benzene 207109-42-0  
207111-02-2 207111-06-6, N-(3-Bromo-4-(methylthio)phenyl)-2,2,2-  
trifluoroacetamide 220982-78-5 220982-79-6 220982-80-9 220982-81-0  
220982-82-1 220982-83-2 220982-84-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT 2252-62-2P 7617-93-8P, 2,5-Bis-trifluoromethylbromobenzene 19056-41-8P  
19432-27-0P, 2-Bromo-4-isopropylphenol 20735-01-7P 20901-65-9P  
31558-30-2P 32445-99-1P, 4-Isopropyl-1-(trifluoromethyl)benzene  
32990-21-9P, Trifluoroacetonitrile oxide 93484-84-5P 190269-55-7P  
190269-57-9P 190269-59-1P 190269-60-4P 190269-69-3P 190269-71-7P  
190269-73-9P 190269-75-1P 190269-76-2P 190269-78-4P 190269-79-5P  
190269-82-0P 190269-90-0P 190271-11-5P 190271-13-7P 191602-40-1P,  
2-Bromo-4-(trifluoroacetamido)anisole 191602-41-2P, 2-Bromo-4-(5-  
(trifluoromethyl)-1H-tetrazol-1-yl)anisole 191602-56-9P 191602-66-1P  
191602-84-3P, 3-Bromo-4-isopropoxybenzaldehyde 200956-13-4P,  
2-Bromo-4-(trifluoromethoxy)phenol 200956-14-5P, 2-Bromo-4-  
(trifluoromethoxy)anisole 206759-09-3P 207110-12-1P 207110-30-3P,  
1-Cyclopropylmethoxy-2-bromo-4-(trifluoromethoxy)benzene 207110-31-4P  
207110-34-7P, 3-Bromo-5-fluoro-4-methyl-1-nitrobenzene 207110-35-8P,  
3-Bromo-5-fluoro-4-methylaniline 207110-36-9P, 3-Bromo-5-fluoro-4-  
methyltrifluoroacetanilide 207110-37-0P 207110-38-1P,  
2-Bromo-1-methoxy-4-(2-methoxyvinyl)benzene 207110-39-2P  
207110-40-5P, 4-(3-Bromo-4-methoxyphenyl)-3-methylisoxazole  
207110-41-6P, 1-(3-Bromo-4-methoxyphenyl)-2,5-dimethylpyrrole  
207110-43-8P 207110-45-0P, 4-(3-Bromo-4-methoxyphenyl)-3-methylpyrazole  
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methylpyrazole 207110-47-2P 207110-48-3P 207110-49-4P 207110-52-9P  
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207110-89-2P 207110-90-5P, 3-(3-Bromo-4-methoxyphenyl)pentane-  
2,4-dione 207110-91-6P 207110-92-7P 207110-93-8P  
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2-Bromo-4-isopropyl-1-(trifluoromethoxy)benzene 207110-98-3P  
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(trifluoromethyl)benzene 207111-96-4P 220982-33-2P 220982-34-3P  
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 2,2-Difluoro-4-bromo-5-(trifluoroacetamide)benzodioxole 220982-75-2P  
 220982-76-3P, 4-(3-Bromo-4-methoxyphenyl)-3-  
 (trifluoromethyl)isoxazole 220982-77-4P, 3-(3-Bromo-4-isopropoxyphenyl)-  
 1,3-pentane-2,4-dione

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor  
 antagonists for treatment of diseases)

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RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);

USES (Uses)

(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor  
 antagonists for treatment of diseases)

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 220982-28-5P 220982-29-6P 220982-30-9P 220982-32-1P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL

(Biological study); PREP (Preparation); USES (Uses)

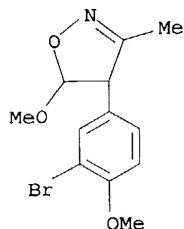
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor  
 antagonists for treatment of diseases)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; WO 9420500 1994 HCAPLUS
- (2) Anon; WO 9620197 1996 HCAPLUS
- (3) Anon; WO 9714671 1997 HCAPLUS
- (4) Anon; WO 9719084 1997 HCAPLUS
- (5) Anon; WO 9730055 1997 HCAPLUS
- (6) Anon; WO 9730056 1997 HCAPLUS
- (7) Anon; WO 9749710 1997 HCAPLUS
- (8) Desai; US 5688806 1997 HCAPLUS
- (9) Mills; US 5387595 1995 HCAPLUS

IT 207110-39-2P  
 RL: SPN (Synthetic preparation); SPN (Synthetic preparation); PREP (Preparation); PREP (Preparation)  
 (preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)  
 RN 207110-39-2 HCAPLUS  
 CN Isoxazole, 4-(3-bromo-4-methoxyphenyl)-4,5-dihydro-5-methoxy-3-methyl- (9CI) (CA INDEX NAME)



L28 ANSWER 9 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:45215 HCAPLUS  
 DN 130:110269  
 ED Entered STN: 22 Jan 1999  
 TI Preparation of isoxazole compounds as cyclooxygenase inhibitors  
 IN Talley, John J.  
 PA G.D. Searle and Co., USA  
 SO U.S., 52 pp., Cont.-in-part of U.S. 5,633,272.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D261-06  
 NCL 548247000  
 CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

## FAN.CNT 3

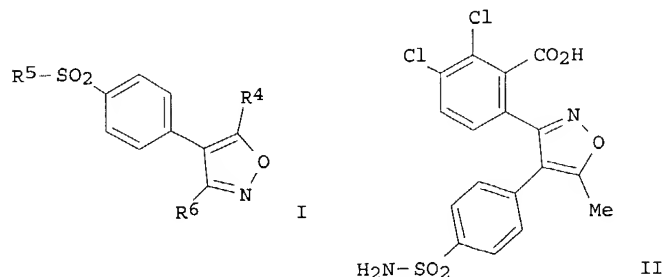
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5859257	A	19990112	US 1996-702417	19960814 <--
	US 5633272	A	19970527	US 1995-473884	19950607 <--
PRAI	US 1995-387680	B2	19950213	<--	
	US 1995-473884	A2	19950607	<--	

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5859257	ICM	C07D261-06
	NCL	548247000

OS CASREACT 130:110269; MARPAT 130:110269

GI



AB Claimed is a method of preparing title compds. I [R4 = alkyl, etc.; R5 = amino; R6 = (un)substituted phenyl] by treatment of a diphenylethanone derivative with hydroxylamine, treating said oxime with base and an acylating agent to form a diphenylisoxazoline derivative, and forming the (isoxazol-4-yl)benzenesulfonamide by treatment of the isoxazoline with chlorosulfonic acid and ammonia. The title compound II in vitro showed IC50

values of 0.4 .mu.M and > 100 .mu.M against COX-2 and COX-1, resp.  
 ST isoxazole prepn cyclooxygenase 2 inhibitor; cyclooxygenase 2 inhibitor  
 isoxazole prepn  
 IT Intestine, disease  
 (inflammatory; preparation and effect of isoxazole compds. with effect on  
 COX-2)  
 IT Analgesics  
 (preparation and effect of isoxazole compds. as cyclooxygenase inhibitors)  
 IT Alzheimer's disease  
 Arthritis  
 (preparation and effect of isoxazole compds. with effect on COX-2)  
 IT Anti-inflammatory agents  
 (preparation of isoxazole compds. as cyclooxygenase inhibitors)  
 IT Intestine, disease  
 (ulcerative colitis; preparation and effect of isoxazole compds. with effect  
 on COX-2)  
 IT 181695-72-7P 181695-73-8P 181695-74-9P  
 181695-75-0P 181695-76-1P 181695-77-2P  
 181695-78-3P 181695-79-4P 181695-80-7P  
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 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); IMF (Industrial manufacture); SPN  
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
 study); PREP (Preparation); USES (Uses)  
 (preparation of isoxazole compds. as cyclooxygenase inhibitors)  
 IT 39391-18-9, Cyclooxygenase  
 RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL  
 (Biological study)  
 (preparation of isoxazole compds. as cyclooxygenase inhibitors)  
 IT 64-17-5, Ethanol, reactions 71-43-2, Benzene, reactions 75-16-1,  
 Methylmagnesium bromide 75-36-5, Acetyl chloride 79-20-9 98-59-9,  
 Toluenesulfonyl chloride 99-76-3, Methyl 4-hydroxybenzoate 100-39-0,  
 Benzyl bromide 100-52-7, Benzaldehyde, reactions 101-41-7, Methyl  
 phenylacetate 103-79-7, Phenylacetone 103-80-0, Phenylacetyl chloride  
 103-82-2, Phenylacetic acid, reactions 104-87-0, p-Tolualdehyde  
 104-88-1, p-Chlorobenzaldehyde, reactions 108-24-7 108-30-5, Succinic  
 anhydride, reactions 108-55-4, Glutaric anhydride 108-89-4 109-72-8,  
 Butyllithium, reactions 110-13-4, Acetonylacetone 123-11-5,  
 4-Anisaldehyde, reactions 124-38-9, Carbon dioxide, reactions  
 321-28-8, 2-Fluoroanisole 358-23-6, Trifluoromethanesulfonic anhydride  
 451-40-1, Desoxybenzoin 459-57-4, 4-Fluorobenzaldehyde 553-90-2,  
 Dimethyl oxalate 587-04-2, 3-Chlorobenzaldehyde 693-03-8,  
 Butylmagnesium bromide 766-51-8, 2-Chloroanisole 925-90-6,  
 Ethylmagnesium bromide 1007-32-5, 1-Phenyl-2-butanone 1122-91-4,  
 4-Bromobenzaldehyde 1336-21-6, Ammonium hydroxide 1722-69-6,  
 1,2-Diphenyl-1-buten-3-one 2466-76-4, N-Acetylhydrazide 2646-90-4,  
 2,5-Difluorobenzaldehyde 2893-05-2 2950-43-8, Hydroxylamine O-sulfonic  
 acid 3446-89-7, 4-(Methylthio)benzaldehyde 3795-79-7, Methyl  
 4-(methylthio)benzoate 4111-54-0, Lithium diisopropylamide 4166-53-4,  
 3-Methylglutaric anhydride 4206-67-1, Trimethylsilyliodomethane  
 4480-83-5, 1,4-Dioxane-2,6-dione 5188-07-8, Sodium thiomethoxide

5470-11-1, Hydroxylamine hydrochloride 6287-38-3, 3,4-Dichlorobenzaldehyde 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6683-92-7, 1-Phenyl-2-pentanone 7446-09-5, Sulfur dioxide, reactions 7664-41-7, Ammonia, reactions 7677-24-9, Trimethylsilylcyanide 7790-94-5, Chlorosulfonic acid 13528-93-3, Bis(1,2-chlorodimethylsilyl)ethane 16188-55-9, 4-(Methylthio)phenylacetic acid 24424-99-5, Di-tert-butyl dicarbonate 34036-07-2, 3,4-Difluorobenzaldehyde 63327-11-7 88356-92-7 104372-31-8 219679-80-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of isoxazole compds. as cyclooxygenase inhibitors)  
 IT 325-62-2P 492-38-6P 952-06-7P 1023-17-2P 1529-41-5P 2001-28-7P  
 2001-29-8P 3475-29-4P 6318-76-9P 6574-99-8P 13721-20-5P  
 16736-09-7P 16736-13-3P 16737-10-3P 25632-70-6P 25870-62-6P  
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 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of isoxazole compds. as cyclooxygenase inhibitors)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; EP 026928 1981 HCAPLUS
- (2) Anon; JP 2223568 1990
- (3) Anon; JP 4173780 1992
- (4) Anon; WO 9219604 1992 HCAPLUS
- (5) Anon; EP 549797 1993 HCAPLUS
- (6) Anon; AU 9335480 1993 HCAPLUS
- (7) Anon; DE 4314966 1994 HCAPLUS
- (8) Anon; EP 623603 1994 HCAPLUS
- (9) Anon; WO 9417059 1994 HCAPLUS
- (10) Anon; WO 9420475 1994 HCAPLUS
- (11) Anon; EP 633254 1995 HCAPLUS
- (12) Anon; WO 9500501 1995 HCAPLUS
- (13) Anon; WO 9512587 1995 HCAPLUS
- (14) Anon; WO 9514672 1995 HCAPLUS
- (15) Descamps; Bull Soc Chim Belg 1964, V73, P459 HCAPLUS
- (16) Hagiwara; US 5310926 1994 HCAPLUS
- (17) Suzuki; US 5318970 1994 HCAPLUS
- (18) Talley; US 5633272 1997 HCAPLUS
- (19) Umezawa; Chem 1963, V36(9), P1150 HCAPLUS
- (20) Yamawaki, I; Chem Pharm Bull 1988, V36, P3142 HCAPLUS

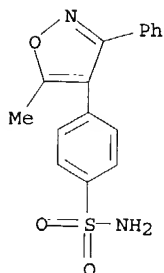
IT 181695-72-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); PREP (Preparation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of isoxazole compds. as cyclooxygenase inhibitors)

RN 181695-72-7 HCAPLUS

CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX NAME)





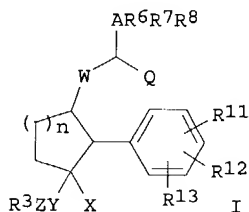
L28 ANSWER 10 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1998:306975 HCAPLUS  
 DN 129:15967  
 ED Entered STN: 25 May 1998  
 TI Preparation of arylcycloalkanes as tachykinin receptor antagonists.  
 IN Caldwell, Charles G.; Chen, Ping; Durette, Philippe L.; Finke, Paul; Hale, Jeffrey; Holson, Edward; Kopka, Ihor; Maccoss, Malcolm; Meurer, Laura; Mills, Sander G.; Robichaud, Albert  
 PA Merck and Co., Inc., USA  
 SO U.S., 109 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A61K031-41  
 ICS C07D257-04; C07D271-10  
 NCL 514364000  
 CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1, 27, 28  
 FAN.CNT 1  

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5750549	A	19980512	US 1996-730277	19961015 <--
PRAI US 1996-730277		19961015 <--		

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5750549	ICM	A61K031-41
	ICS	C07D257-04; C07D271-10
	NCL	514364000

  
 OS MARPAT 129:15967  
 GI



AB Title compds. [I; R3 = H, alkoxy, phenylalkoxy, Ph, cyano, halo, amino, (substituted) alkyl, null; R6-R8 = H, alkoxy, halo, (substituted) alkyl, OH, cyano, CF3, NO2, heterocyclyl, etc.; R11-R13 = H, (substituted) alkyl, halo, cyano, CF3, NO2, OH, alkoxy, etc.; A = Ph, benzofuranyl, benzothienophenyl, benzothiazoyl, indolyl, imidazolyl, oxadiazolyl, pyridyl, pyrimidyl, quinolinyl, thiazolyl, thienyl, thiophenyl, dihydrobenzofuranyl; Q = H, alkyl; W = O, NH, alkylimino, NHCO, alkyliminocarbonyl; X = H, alkyl; Y = bond, (substituted) alkyl; Z = NR15, CONR15, SO2NR15, SO2, CO2R15, CH2OR15, null; R15 = H, (substituted) alkyl; n = 1-3; with provisos], were prepared Thus, Me 3(SR)-hydroxy-2(RS)-phenylcyclopentane-1(RS)-carboxylate (preparation given) was treated with 3,5-bis(trifluoromethyl)benzyl bromide and NaH in DMF to give Me 3(SR)-[3,5-bis(trifluoromethyl)phenylmethoxyl]-2(RS)-phenylcyclopentane-1(RS)-carboxylate. I showed intrinsic tachykinin receptor antagonist activity in the range 0.05-10 .mu.M.

ST arylcycloalkane prepn tachykinin receptor antagonist; substance P  
antagonist arylcycloalkane prepn

IT Nerve, disease  
(diabetic neuropathy, treatment; preparation of arylcycloalkanes as  
tachykinin receptor antagonists)

IT Nerve, disease  
(neuralgia, treatment; preparation of arylcycloalkanes as tachykinin  
receptor antagonists)

IT Nerve, disease  
(neuropathy, treatment; preparation of arylcycloalkanes as tachykinin  
receptor antagonists)

IT Nerve, disease  
(peripheral neuropathy, treatment; preparation of arylcycloalkanes as  
tachykinin receptor antagonists)

IT Analgesics  
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT Cystic fibrosis  
(treatment; preparation of arylcycloalkanes as tachykinin receptor  
antagonists)

IT 33507-63-0P, Substance P 86933-74-6P, Neurokinin A  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(antagonists; preparation of arylcycloalkanes as tachykinin receptor  
antagonists)

IT 190268-90-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of)

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190269-02-4P 190269-05-7P 190269-10-4P 190269-11-5P 190269-12-6P  
190269-15-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 190269-17-1P 190269-19-3P 190269-21-7P 190269-22-8P 190269-23-9P  
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207730-70-9P 207730-71-0P 207730-73-2P 207730-74-3P 207730-83-4P  
207730-89-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 70-23-5, Ethyl bromopyruvate 75-16-1, Methylmagnesium bromide 75-30-9,  
2-Iodopropane 79-22-1, Methyl chloroformate 79-44-7, Dimethylcarbamoyl  
chloride 100-52-7, Benzaldehyde, reactions 105-56-6, Ethyl  
cyanoacetate 109-04-6, 2-Bromopyridine 123-75-1, Pyrrolidine,  
reactions 144-48-9, Iodoacetamide 288-32-4, Imidazole, reactions  
459-57-4, 4-Fluorobenzaldehyde 609-71-2, 2-Hydroxy-3-carboxypyridine  
624-83-9, Methyl isocyanate 624-84-0, Formic hydrazide 626-55-1,  
3-Bromopyridine 635-21-2, 2-Chloro-5-aminobenzoic acid 785-56-8,  
3,5-Bis(trifluoromethyl)benzoyl chloride 874-60-2, 4-Methylbenzoyl  
chloride 1066-54-2, Trimethylsilylacetylene 1515-78-2,  
1-Phenyl-1,3-butadiene 1761-61-1, 5-Bromosalicylaldehyde 1765-93-1,  
4-Fluorobenzeneboronic acid 1779-49-3, Methyltriphenylphosphonium  
bromide 2362-61-0 2393-23-9, 4-Methoxybenzylamine 2941-72-2,  
6-Methoxy-2-methylbenzothiazole 3034-55-7, 5-Bromothiazole 4405-13-4,  
Glyoxal trimer dihydrate 4892-02-8, Methyl thiosalicylate 5292-43-3,  
tert-Butyl bromoacetate 6165-68-0, Thiophene-2-boronic acid 6482-24-2,  
2-Methoxyethyl bromide 6959-48-4, 3-Picolyl chloride hydrochloride  
7252-83-7, Bromoacetaldehyde dimethyl acetal 7531-52-4, L-Prolineamide  
14006-51-0, 3-Methoxybenzo[b]thiophene-2-carboxaldehyde 25016-01-7  
30071-93-3 32247-96-4, 3,5-Bis(trifluoromethyl)benzyl bromide  
34259-99-9, 4-Bromothiazole 35134-07-7, 3-Methoxythiophene-2-  
carboxaldehyde 36805-97-7, N,N-Dimethylformamide di-tert-butyl acetal  
67868-79-5 68236-21-5 72479-05-1 82069-74-7, 3-Methoxythiophene-4-  
carboxaldehyde 89378-75-6 90719-27-0 92623-00-2 98273-19-9,  
2-Methoxycarbonyl-4,6-dichloropyridine 119795-13-0 121124-97-8,  
3-Formyl-4-methoxyphenylboronic acid 145742-65-0 155742-64-6  
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170729-89-2 172480-83-0 175205-84-2 175277-50-6 180574-24-7  
190269-95-5 190270-88-3 190270-91-8, 6-Methoxy-2-methylbenzothiazole-7-  
carboxaldehyde 190271-57-9 190271-65-9 190271-66-0 190271-67-1  
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3-Methoxyquinolin-2-carboxaldehyde 190271-73-9 190271-74-0  
190271-75-1 190271-77-3 190271-78-4, 5-Methoxycarbonyl-2-  
isopropoxybenzaldehyde 190271-79-5, 5-Aminocarbonyl-2-  
isopropoxybenzaldehyde 190271-80-8 190271-81-9 190271-82-0  
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RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 368-63-8P 3704-28-7P, Methyl 2-methylthiobenzoate 6854-07-5P,  
2-Hydroxy-3-carboxy-5-nitropyridine 33384-77-9P, 2-(Methylthio)benzyl  
alcohol 38185-19-2P 42122-75-8P 53606-06-7P, 2-  
(Methylsulfonyl)benzyl bromide 122433-50-5P 122433-51-6P  
132683-62-6P, 2-Formyl-4,6-dichloropyridine 138505-25-6P,  
5-Bromo-2-isopropoxybenzaldehyde 145742-56-9P 160376-84-1P  
163257-19-0P 163257-23-6P 168267-13-8P 190268-01-0P 190268-07-6P  
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of arylcycloalkanes as tachykinin receptor antagonists)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; EP 0142322 1985 HCAPLUS
- (2) Anon; EP 0436334 A2 1991 HCAPLUS
- (3) Anon; WO 9300331 1993 HCAPLUS
- (4) Anon; WO 9400440 1994 HCAPLUS
- (5) Anon; WO 9515311 1995 HCAPLUS
- (6) Anon; WO 9516679 1995 HCAPLUS
- (7) Anon; Chemical Abstracts 1966, V64(8), P12732
- (8) Baker; US 5444074 1995 HCAPLUS
- (9) Baker; US 5496833 1996 HCAPLUS
- (10) Braus; US 3574165 1971 HCAPLUS
- (11) Dorn; US 5512570 1996 HCAPLUS
- (12) Mills; US 5387595 1995 HCAPLUS
- (13) Miura; US 4755617 1988 HCAPLUS
- (14) Seward; US 5561130 1996 HCAPLUS
- (15) Williams; US 5459270 1995 HCAPLUS

IT 190268-23-6P

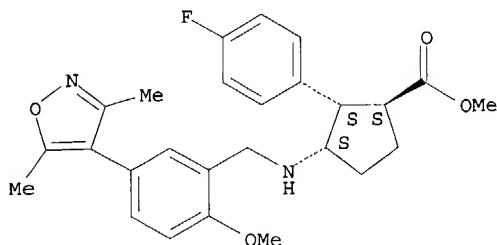
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation);  
 USES (Uses)

(preparation of arylcycloalkanes as tachykinin receptor antagonists)

RN 190268-23-6 HCAPLUS

CN Cyclopentanecarboxylic acid, 3-[[[5-(3,5-dimethyl-4-isoxazolyl)-2-  
 methoxyphenyl]methyl]amino]-2-(4-fluorophenyl)-, methyl ester,  
 monohydrochloride, (1R,2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

L28 ANSWER 11 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1997:372654 HCAPLUS  
 DN 127:65756  
 ED Entered STN: 14 Jun 1997  
 TI Preparation of substituted isoxazoles for the treatment of inflammation  
 IN Talley, John J.; Brown, David L.; Nagarajan, Srinivasan; Carter, Jeffery  
 S.; Weier, Richard M.; Stealey, Michael A.; Collins, Paul W.; Rogers,  
 Roland S.; Seibert, Karen  
 PA USA  
 SO U.S., 28 pp., Cont.-in-part of U.S. Ser. No. 387,680, abandoned.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D261-06  
 ICS C07D261-10; C07D261-12; C07D261-14; A61K031-42  
 NCL 514378000  
 CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

FAN.CNT 3

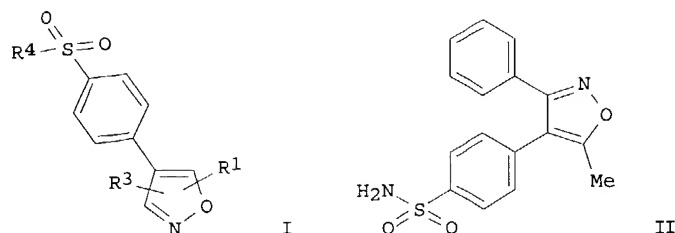
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5633272	A	19970527	US 1995-473884	19950607 <--
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CA 2212836	C	20030812		
WO 9625405	A1	19960822	WO 1996-US1869	19960212 <--
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RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR				
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AU 699593	B2	19981210		
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EP 809636	A1	19971203	EP 1996-904614	19960212 <--
EP 809636	B1	20020904		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
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CN 1107058	B	20030430		
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JP 3267300	B2	20020318		
JP 2002179656	A2	20020626	JP 2001-326343	19960212 <--
EP 1223167	A2	20020717	EP 2002-3253	19960212 <--
EP 1223167	A3	20020807		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
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PT 809636	T	20021231	PT 1996-904614	19960212 <--
RU 2200158	C2	20030310	RU 1997-115452	19960212 <--
ES 2183935	T3	20030401	ES 1996-904614	19960212 <--
PL 185510	B1	20030530	PL 1996-321814	19960212 <--
PL 185544	B1	20030530	PL 1996-351239	19960212 <--
CZ 293211	B6	20040317	CZ 1997-2546	19960212 <--
ZA 9601150	A	19970212	ZA 1996-1150	19960213 <--
TW 449587	B	20010811	TW 1996-85109684	19960809 <--
US 5859257	A	19990112	US 1996-702417	19960814 <--
US 5985902	A	19991116	US 1997-801768	19970218 <--
FI 9703292	A	19970811	FI 1997-3292	19970811 <--
NO 9703711	A	19971006	NO 1997-3711	19970812 <--
CN 1442139	A	20030917	CN 2003-107042	20030228 <--
PRAI US 1995-387680	B2	19950213	<--	
US 1995-473884	A	19950607	<--	
EP 1996-904614	A3	19960212	<--	
JP 1996-525057	A3	19960212	<--	
WO 1996-US1869	W	19960212	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5633272	ICM	C07D261-06
	ICS	C07D261-10; C07D261-12; C07D261-14; A61K031-42
	NCL	514378000

OS MARPAT 127:65756

GI

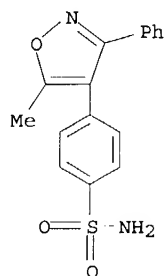


- AB The title compds. [I; R1 = alkyl, carboxyalkyl, alkoxyalkyl, etc.; R3 = (un)substituted cycloalkyl, cycloalkenyl, aryl; R4 = lower alkyl, OH, NH2], useful in treatment of inflammation and inflammation-associated disorders such as arthritis, pain, and fever, were prepared Thus, treatment of desoxybenzoin oxime with BuLi/hexanes in THF followed by addition of Ac2O, reaction of the resulting 3,4-diphenyl-4-hydroxy-5-methylisoxazole with ClSO3H, and treatment of the intermediate with saturated NH4OH solution afforded 30% II which showed ID50 of < 0.1 .mu.M against COX-2.
- ST isoxazole prepn antiinflammatory; antiarthritic isoxazole prepn; analgesic isoxazole prepn; antipyretic isoxazole prepn; cyclooxygenase inhibitor isoxazole prepn
- IT Analgesics  
Anti-inflammatory agents  
Antiarthritics  
Antipyretics  
(preparation of substituted isoxazoles for the treatment of inflammation)
- IT 39391-18-9  
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)  
(COX-2 inhibitors; preparation of substituted isoxazoles for the treatment of inflammation)
- IT 181695-72-7P 181695-81-8P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of substituted isoxazoles for the treatment of inflammation)
- IT 181695-73-8P 181695-74-9P 181695-75-0P  
181695-76-1P 181695-78-3P 181695-79-4P  
181695-80-7P 181695-82-9P 181695-83-0P  
181695-84-1P 181696-24-2P 181696-25-3P  
181696-26-4P 181696-27-5P 181696-28-6P  
181696-29-7P 181696-30-0P 181696-31-1P  
181696-32-2P 181696-33-3P 181696-34-4P  
181696-35-5P 181696-36-6P 181696-37-7P  
181696-38-8P 181696-39-9P 181696-40-2P  
181696-41-3P 181696-42-4P 181696-43-5P  
181696-44-6P 181696-45-7P 191421-97-3P  
191421-98-4P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of substituted isoxazoles for the treatment of inflammation)
- IT 71-43-2, Benzene, reactions 103-80-0, Phenylacetyl chloride 108-30-5, Succinic anhydride, reactions 321-28-8, 2-Fluoroanisole 451-40-1, Desoxybenzoin 766-51-8, 2-Chloroanisole 1722-69-6, 1,2-Diphenyl-1-buten-3-one 3446-89-7, 4-Methylthiobenzaldehyde 63327-11-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of substituted isoxazoles for the treatment of inflammation)
- IT 325-62-2P 952-06-7P 3475-29-4P 13721-20-5P, 3-Chloro-4-methoxyphenylacetic acid 25632-70-6P 37612-52-5P 37928-17-9P  
78967-09-6P 177560-74-6P 181696-73-1P 181696-74-2P  
181696-75-3P 181696-76-4P 181696-77-5P  
181696-78-6P 181696-80-0P 181696-81-1P 181696-82-2P  
181696-83-3P 181696-84-4P 181696-85-5P 181696-86-6P  
181696-87-7P 181696-89-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of substituted isoxazoles for the treatment of inflammation)
- IT 181695-72-7P

RL: BAC (Biological activity or effector, except adverse); SPN  
 (Synthetic preparation); PREP (Preparation); SPN  
 (Synthetic preparation); THU (Therapeutic use); PREP  
 (Preparation); PREP (Preparation); RACT (Reactant or  
 reagent); USES (Uses)  
 (preparation of substituted isoxazoles for the treatment of inflammation)

RN 181695-72-7 HCAPLUS

CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX  
 NAME)



L28 ANSWER 12 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:70248 HCAPLUS

DN 126:144549

ED Entered STN: 31 Jan 1997

TI Preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta.  
 converting enzyme inhibitors

IN Dolle, Roland E.; Singh, Jasbir; Whipple, David A.; Prouty, Catherine;  
 Chaturvedula, Prasad V.; Schmidt, Stanley J.; Awad, Mohamed M. A.; Hoyer,  
 Denton W.; Ross, Tina M.

PA Sanofi Winthrop Inc., USA

SO U.S., 17 pp., Cont.-in-part of U.S. Ser. No. 237, 920, abandoned.

CODEN: USXXAM

DT Patent

LA English

IC ICM A61K038-00

ICS A61K031-415; C07K005-00; C07D231-04

NCL 514018000

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 63

FAN.CNT 3

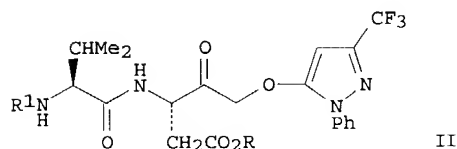
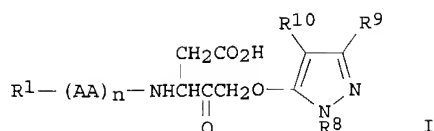
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PI	US 5585357	A	19961217	US 1996-593773	19960129 <--
	JP 07089951	A2	19950404	JP 1994-119873	19940601 <--
	CA 2125021	AA	19941204	CA 1994-2125021	19940602 <--
	AU 9463473	A1	19950427	AU 1994-63473	19940602 <--
	AU 690102	B2	19980423		
	IL 109867	A1	19980715	IL 1994-109867	19940602 <--
	FI 9402624	A	19941204	FI 1994-2624	19940603 <--
	NO 9402064	A	19941205	NO 1994-2064	19940603 <--
	HU 68689	A2	19950728	HU 1994-1679	19940603 <--
	HU 75964	A2	19970528	HU 1996-2985	19950428 <--
	US 5677283	A	19971014	US 1996-732173	19961016 <--
PRAI	US 1993-71623		19930603	<--	
	US 1994-237920		19940429	<--	
	US 1994-236425		19940429	<--	
	US 1996-593773		19960129	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5585357	ICM	A61K038-00
	ICS	A61K031-415; C07K005-00; C07D231-04
	NCL	514018000

OS MARPAT 126:144549

GI



- AB Title compds. I [each AA = independently L-Val, L-Ala; N-methylalanine, N-methylvaline; R1 = 4-Me2NCH2C6H4CO, PhCH2O2C (Z), PhCH2CO, (4-pyridylmethyl)carbonyl, 3-piperidinopropionyl, 4-(morpholinoethoxy)benzoyl, 2-quinuclidinylcarbonyl, (3-pyridyl)methoxycarbonyl, (2-pyridyl)methoxycarbonyl, (4-phenylpiperazino)carbonyl; R8, R9, R10 = independently H, lower alkyl, halo-substituted Me, carbalkoxy, PhCH2, Ph, or Ph mono or disubstituted with F, NO2, MeO, Cl, CF3, MeSO2] which inhibit interleukin-1.β. protease activity, pharmaceutical compns. containing the compds. and methods using the compds. are provided (no data). Thus, substitution of protected dipeptide bromomethyl ketone Z-L-Val-L-Asp(OCMe3)-CH2Br with 1-phenyl-3-trifluoromethyl-5-pyrazolone gave ester II (R = CMe3, R1 = Z) in 85% yield. Hydrogenolysis of the Z group, acylation with 4-(Me2NCH2)C6H4COCl, and acidic deesterification gave title compound II [R = H, R1 = 4-(Me2NCH2)C6H4CO] in 50% yield.
- ST peptidyl heteroaryloxymethyl ketone prepn enzyme inhibitor; interleukin converting enzyme inhibitor heteroaryloxymethyl ketone
- IT Ketones, preparation  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (peptidyl, heteroaryloxymethyl; preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.β. converting enzyme inhibitors)
- IT 9001-92-7, Protease  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (Interleukin-1.β.; preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.β. converting enzyme inhibitors)
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| IT | 159391-12-5P | 159391-13-6P | 159391-14-7P | 159391-18-1P | 159391-21-6P |
|    | 168318-05-6P | 168318-06-7P | 168318-07-8P | 168318-08-9P | 168318-10-3P |
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|    | 168318-17-0P | 168318-18-1P | 168318-19-2P | 168318-20-5P | 168318-21-6P |
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|    | 168318-28-3P | 168318-29-4P | 168318-30-7P | 168318-32-9P | 168318-34-1P |
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|    | 168318-43-2P | 168318-45-4P | 168318-46-5P | 168318-47-6P | 168318-48-7P |
|    | 168318-49-8P | 168318-51-2P | 168318-52-3P | 168318-53-4P | 168318-54-5P |
|    | 168318-55-6P | 168318-56-7P | 168318-57-8P | 168318-60-3P | 168318-61-4P |
|    | 168318-62-5P | 168318-63-6P | 168318-64-7P | 168318-65-8P | 168318-66-9P |
|    | 168318-67-0P | 168318-68-1P | 168318-69-2P | 168318-72-7P | 168318-73-8P |
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|    | 168318-79-4P | 168318-80-7P | 168318-82-9P | 168318-85-2P | 168318-86-3P |
|    | 168318-87-4P | 168318-88-5P | 168318-89-6P | 168318-93-2P | 168318-94-3P |
|    | 186498-14-8P | 186498-51-1P | 186498-52-2P | 186498-53-3P | 186498-54-4P |
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|    | 186498-60-2P | 186498-61-3P | 186498-62-4P | 186498-63-5P | 186498-64-6P |
|    | 186498-65-7P | 186498-66-8P | 186498-67-9P | 186498-68-0P |              |
|    | 186498-69-1P |              |              |              |              |
- RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.β. converting enzyme inhibitors)
- IT 321-07-3, 1-Phenyl-3-trifluoromethyl-5-pyrazolone 1076-38-6,



4-Hydroxycoumarin 1786-05-6, 4-Hydroxy-3-phenylcoumarin 16854-67-4,  
4-Hydroxythiocoumarin 18469-52-8, Methyl 4-(aminomethyl)benzoate  
21474-06-6, 4-Hydroxy-3-phenylisoxazole 23253-51-2, 5-Hydroxy-3-  
phenylisoxazole 27772-79-8 89819-63-6, 5-Hydroxy-3-(4-  
pyridinyl)isoxazole 134581-47-8 168319-04-8 168319-05-9  
168319-06-0 186498-70-4 186498-72-6 186498-73-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta.  
converting enzyme inhibitors)

IT 18364-71-1P 121811-18-5P, 4-(N,N-Dimethylaminomethyl)benzoyl chloride  
168318-98-7P 168318-99-8P 168319-00-4P 168319-01-5P 168319-02-6P  
186498-71-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta.  
converting enzyme inhibitors)

IT 186498-66-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation);

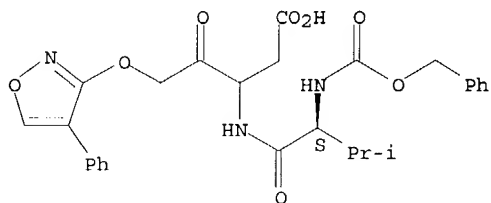
USES (Uses)

(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta.  
converting enzyme inhibitors)

RN 186498-66-8 HCAPLUS

CN Pentanoic acid, 3-[[3-methyl-1-oxo-2-[[[(phenylmethoxy)carbonyl]amino]butyl  
]amino]-4-oxo-5-[(4-phenyl-3-isoxazolyl)oxy]-, [3(S)]- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.



L28 ANSWER 13 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:52859 HCAPLUS

DN 124:261059

ED Entered STN: 26 Jan 1996

TI Pyridazine derivatives useful as ligands of muscarinic cholinergic  
receptors

IN Boigegrain, Robert; Brodin, Roger; Kan, Jean P.; Olliero, Dominique;  
Bourguignon, Jean Jacques; Worms, Paul

PA Sanofi, Fr.

SO U.S., 28 pp. Cont.-in-part of U.S. Ser. No. 737, 654, abandoned.

CODEN: USXXAM

DT Patent

LA English

IC A61K031-50

NCL 514247000

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5461053	A	19951024	US 1992-964901	19921022 <--
	FR 2642754	A1	19900810	FR 1989-1547	19890207 <--
	FR 2642754	B1	19910524		
	FR 2642757	A1	19900810	FR 1989-1548	19890207 <--
	FR 2642757	B1	19910524		
	FR 2654727	A1	19910524	FR 1989-15137	19891117 <--
	FR 2654727	B1	19920327		
	FR 2663326	A2	19911220	FR 1990-7533	19900615 <--
	FR 2663326	B2	19921016		
	FR 2665442	A1	19920207	FR 1990-9777	19900731 <--
	FR 2665442	B1	19921204		
	FI 9005663	A	19910518	FI 1990-5663	19901115 <--
	ZA 9009221	A	19910925	ZA 1990-9221	19901116 <--
	US 5631255	A	19970520	US 1995-473582	19950607 <--

Searched by Noble Jarrell

US 5656631	A	19970812	US 1995-473580	19950607 <--
PRAI FR 1989-1547		19890207	<--	
FR 1989-1548		19890207	<--	
FR 1989-15137		19891117	<--	
US 1990-475489		19900207	<--	
FR 1990-7533		19900615	<--	
FR 1990-9777		19900731	<--	
US 1990-615373		19901119	<--	
US 1991-737654		19910730	<--	
US 1992-871505		19920421	<--	
US 1992-964901		19921022	<--	

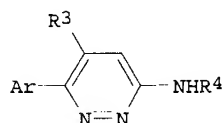
## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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US 5461053	IC	A61K031-50
	NCL	514247000

OS MARPAT 124:261059

GI



AB The present invention relates to pyridazine derivs. I in which: Ar represents a Ph group substituted by R1 and R2 ; R1 and R2 each independently denotes hydrogen, halogen, trifluoromethyl, hydroxyl, C1-C4 alkoxy or C1-C4 alkyl; R3 represents C3H7, C3-C7 cycloalkyl or the Ar' radical, Ar' being Ph substituted by R1 and R2 ; R4 represents the group CH2C(CH2X1)2(CH2)nNR5R6 in which: X1 represents hydrogen or methyl; n is 0; R5 represents a C1-C6 linear alkyl group; and R6 represents a C1-C6 linear alkyl group; or a group Alk-NR5aR6a in which Alk is a C1-C6 linear alkylene group, R5a is hydrogen or a C1-C6 alkyl group and R6a alkyl group, a benzyl or a C3-C7 cycloalkyl, with the proviso that R1 and R2 are not simultaneously H when Alk is (CH2)2, and that R4 is the group AlkNR5aR6a only when R3 is a C3H7 or a Ph group; or its salts, which are pharmaceutically acceptable or permit suitable separation or crystallization thereof, which are useful as ligands of cholinergic receptors, in particular, receptors of the M1 type. Thus, e.g., amination of 6-chloro-3-phenyl-4-propylpyridazine (preparation given) with 2-(dimethylamino)-2-methylpropylamine (preparation given) afforded a base which was converted to 3-(2-diethylamino-2-methylpropyl)amino-6-phenyl-5-propyl-pyridazine sesquifumarate (SR 46559A); SR 46559A exhibited IC50's of 0.11 and 2.2 .mu.mol, resp., representing affinity for M1 and M2 muscarinic cholinergic receptors. Pharmaceutical formulations were given.

ST pyridazine deriv ligand muscarinic cholinergic receptor

IT Nervous system

(central, cholinergic, disease, deficiency, treatment; pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT Receptors

RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)

(muscarinic M1, pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 132449-99-1P, SR 96185 132450-00-1P 132450-01-2P, SR 96194A  
 132450-02-3P, SR 96181 132450-03-4P, SR 96198 132450-04-5P, SR 96222  
 132450-05-6P, SR 46004A 132450-06-7P, SR 96204A 132450-07-8P, SR  
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 SR 45988A 132450-53-4P, SR 45989A 132450-54-5P, SR 46377A

132450-56-7P, SR 46532A 132450-57-8P, SR 46728A 132450-59-0P, SR  
 96290A 132450-60-3P, SR 96291 132450-62-5P, SR 46352A 132450-64-7P,  
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 132450-74-9P, SR 96269 132450-75-0P, SR 96272 132450-76-1P, SR 46433  
 132450-77-2P, SR 46434 132450-78-3P, SR 46430 132450-80-7P, SR 47046  
 132450-82-9P, SR 47186 132450-84-1P, SR 47226 132450-85-2P, SR 96305  
 132450-87-4P, SR 96307A 132450-88-5P, SR 96308A 132450-90-9P, SR  
 46457A 132450-92-1P, SR 46578A 132450-94-3P, SR 46640A 132471-76-2P,  
 SR 46082A 132471-78-4P, SR 46730A 132471-79-5P, SR 96306A  
 136549-27-4P, SR 46729A 136549-29-6P, SR 46733A 136549-30-9P, SR  
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 47068 136549-38-7P, SR 47069A 136549-40-1P, SR 47227A 136549-41-2P,  
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 136549-48-9P, SR 48081A 136549-49-0P, SR 48082 136549-50-3P, SR 47674A  
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 174756-84-4P, SR 47098A 174794-12-8P, SR 47153A 174794-13-9P, SR 96268  
 174794-14-0P, SR 46641A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 75-86-5, Acetone cyanohydrin 93-55-0, Propiophenone 100-36-7,  
 N,N-Diethylethylenediamine 105-54-4, Ethyl butyrate 109-89-7,  
 reactions 115-11-7, reactions 121-97-1 459-22-3,  
 (4-Fluorophenyl)acetonitrile 924-44-7, Ethyl glyoxylate 1009-14-9,  
 Valerophenone 26116-12-1, 2-(Aminomethyl)-1-ethylpyrrolidine  
 132451-09-3, 3-Chloro-6-(2-methoxyphenyl)-5-methylpyridazine  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 3378-38-9P 21404-84-2P, 2-Diethylamino-2-methylpropionamide  
 21404-89-7P, 2-Diethylamino-2-methylpropylamine 27062-58-4P  
 33048-55-4P, 5-Methyl-6-phenyl-2H-pyridazin-3-one 35672-46-9P,  
 2-Diethylamino-2-methylpropionitrile 66549-28-8P 67820-83-1P  
 68415-28-1P 70777-03-6P 108302-59-6P 127867-89-4P,  
 5-Methyl-6-(4-methoxyphenyl)-2H-pyridazin-3-one 132450-98-7P  
 132450-99-8P 132451-00-4P 132451-01-5P 132451-02-6P 132451-03-7P  
 132451-04-8P 132451-05-9P 132451-06-0P 132451-07-1P 132451-08-2P  
 132451-10-6P 132451-11-7P 132451-12-8P 136549-25-2P 136549-34-3P,  
 6-Phenyl-5-propyl-2H-pyridazin-3-one 136549-51-4P 136549-52-5P  
 136549-53-6P 136549-54-7P 136549-55-8P 136549-56-9P 136549-57-0P  
 136549-58-1P 136549-59-2P 136549-60-5P 136549-61-6P 136549-62-7P  
 136549-63-8P 136549-64-9P 136549-65-0P 136549-66-1P 141235-14-5P,  
 1-(4-Fluorophenyl)pentan-2-one 141235-16-7P 141235-18-9P  
 141235-19-0P 141235-20-3P 141235-21-4P 141235-22-5P 141235-23-6P  
 141235-24-7P 141235-25-8P 141235-26-9P 141235-27-0P 141235-28-1P  
 141235-29-2P 141235-30-5P 141235-31-6P 141235-32-7P 141235-33-8P  
 141235-34-9P 141235-35-0P 141235-36-1P 141235-37-2P 141235-38-3P  
 141235-39-4P 141235-40-7P 141235-41-8P 141235-42-9P 141235-43-0P  
 141235-44-1P 141235-45-2P 141235-46-3P 141235-47-4P 141235-48-5P  
 141235-49-6P 141235-50-9P 141235-51-0P 174700-28-8P 174700-30-2P  
 174700-36-8P, .alpha.-Butyryl-(4-fluorophenyl)acetonitrile

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 174700-36-8P, .alpha.-Butyryl-(4-fluorophenyl)acetonitrile

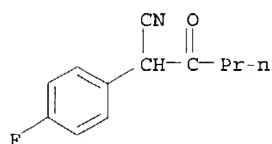
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

RN 174700-36-8 HCAPLUS

CN Benzeneacetonitrile, 4-fluoro-.alpha.-(1-oxobutyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 14 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:931617 HCAPLUS  
 DN 124:146130  
 ED Entered STN: 21 Nov 1995  
 TI [Alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium  
 independent c-AMP phosphodiesterase inhibitor antidepressants  
 IN Saccomano, Nicholas A.; Vinick, Fredric J.  
 PA Pfizer Inc., USA  
 SO U.S., 29 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D239-36  
 ICS A61K031-505  
 NCL 514274000  
 CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 27, 63

## FAN.CNT 2

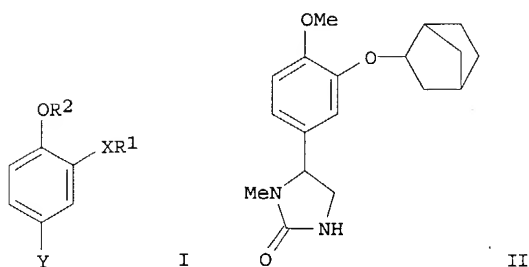
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PI	US 5459145	A	19951017	US 1988-155932	19880119 <--
	US 5128358	A	19920707	US 1991-696690	19910530 <--
	US 5196426	A	19930323	US 1992-854136	19920319 <--
	US 5294730	A	19940315	US 1992-984190	19921120 <--
	US 5414127	A	19950509	US 1994-184092	19940119 <--
PRAI	US 1988-155932	A3	19880119	<--	
	US 1991-696690	A3	19910830	<--	
	US 1992-854136	A3	19920319	<--	
	US 1992-984190	A3	19921120	<--	

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5459145	ICM	C07D239-36
	ICS	A61K031-505
	NCL	514274000
US 5459145	ECLA	C07C217/60; C07C255/37; C07D233/32; C07D233/42; C07D233/78; C07D239/10B; C07D239/22D1; C07D029/36B; C07D285/08B; C07D285/10B; C07D487/04; C07D487/04 <--

OS MARPAT 124:146130

GI



AB Title compds. I wherein R1 is selected from the group consisting of bicyclo[2.2.1]heptyl, bicyclo[2.2.2]octyl, bicyclo[3.2.1]octyl, tricyclo[5.2.1.0<sup>2,6</sup>]decyl, tricyclo[3.3.1.1<sup>3,7</sup>]decyl and indanyl; R2 is Me or Et, X is O or NH; and Y comprises a 5- or 6-membered heterocyclic ring having one or two nitrogens; or fused bicyclic heterocyclic rings having a total of three nitrogen atoms, one in each ring and one angular nitrogen

(no data for antidepressant activity) are prepared as antidepressant agents (no data). Thus, e.g., treatment of 3-(bicyclo[2.2.1]hept-2-yloxy)-4-methoxybenzaldehyde (7:3 endo:exo mixture, preparation given) with NaCN/methylamine hydrochloride afforded a 7:3 endo:exo mixture of cyanoamines; the latter were reduced to 2-methylamino-2-[3-(bicyclo[2.2.1]hept-2-yloxy)-4-methoxyphenyl]ethylamine as a 7:3 endo to exo mixture and cyclized to 1-methyl-5-[3-(bicyclo[2.2.1]hept-2-yloxy)-4-methoxyphenyl]-2-imidazolidinone (II; 17.8%).

ST polycycloalkyloxyphenylheterocyclic calcium independent cAMP phosphodiesterase inhibitor; antidepressant polycycloalkyloxyphenylheterocycle; heterocycle polycycloalkyloxyphenyl antidepressant; polycycloalkylaminophenylheterocyclic calcium independent cAMP phosphodiesterase inhibitor

IT Antidepressants

(([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 115897-70-6P 115897-84-2P 115897-98-8P 115898-36-7P 144034-03-7P  
144034-05-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 115897-71-7P 115897-73-9P 115897-74-0P 115897-75-1P 115897-76-2P  
115897-77-3P 115897-80-8P 115897-83-1P 115897-87-5P 115897-90-0P  
115897-93-3P 115897-96-6P 115897-97-7P 115898-00-5P 115898-05-0P  
115898-06-1P 115898-07-2P 115898-08-3P 115898-19-6P 115898-23-2P  
115898-24-3P 115898-25-4P 115898-26-5P 115898-29-8P 115898-30-1P  
115898-34-5P 115919-88-5P 144033-88-5P 144033-96-5P 144033-97-6P  
144033-98-7P 144033-99-8P 144034-00-4P 144034-06-0P 144034-07-1P  
173252-99-8P 173253-00-4P 173253-01-5P 173253-02-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 9036-21-9, c-AMP phosphodiesterase

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 64-04-0, Phenethylamine 105-53-3, Diethyl malonate 120-80-9,  
Pyrocatechol, reactions 372-09-8, Cyanoacetic acid 497-36-9,  
Endo-Bicyclo[2.2.1]heptan-2-ol 497-38-1, Norcamphor 542-69-8,  
1-Iodobutane 621-59-0, Isovanillin 700-57-2, 2-Adamantanol 931-64-6,  
Bicyclo[2.2.2]-2-octene 1702-10-9 1820-80-0, 3-Aminopyrazole  
2534-77-2, exo-2-Bromonorbornane 5762-56-1, Tris(dimethylamino)methane  
6351-10-6, 1-Indanol 7374-90-5 13380-89-7, Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-  
ol 13380-94-4, Tricyclo[5.2.1.0<sup>2,6</sup>]decan-8-one 29804-62-4,  
Bicyclo[3.2.1]octan-3-ol 31680-08-7, 4-Methoxy-3-nitrobenzaldehyde  
42383-61-9, 2-Aminoimidazole sulfate 50447-20-6 94277-20-0  
113034-45-0 115898-77-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

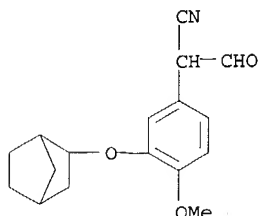
IT 18684-63-4P, Bicyclo[2.2.2]octan-2-ol 56137-56-5P 115897-62-6P  
115897-63-7P 115897-65-9P 115897-66-0P 115897-67-1P 115897-69-3P  
115897-78-4P 115897-79-5P 115897-81-9P 115897-82-0P 115897-85-3P  
115897-86-4P 115897-88-6P 115897-89-7P 115897-91-1P 115897-92-2P  
115897-94-4P 115897-95-5P 115897-99-9P 115898-01-6P  
115898-02-7P 115898-03-8P 115898-04-9P 115898-09-4P  
115898-10-7P 115898-11-8P 115898-12-9P 115898-16-3P 115898-17-4P  
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115898-50-5P 115898-51-6P 115898-52-7P 115898-53-8P 115898-54-9P  
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115898-62-9P 115898-63-0P 115898-64-1P 115898-65-2P 115898-66-3P  
115898-67-4P 115898-68-5P 115898-69-6P 115898-70-9P 115898-71-0P  
115898-72-1P 115898-73-2P 115898-74-3P 115898-75-4P 115898-76-5P  
115898-78-7P 115919-89-6P 131408-38-3P 131408-40-7P 131486-67-4P  
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173252-98-7P 173327-35-0P 173327-36-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium

independent c-AMP phosphodiesterase inhibitor antidepressants)  
 IT 115898-01-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 ([alkoxy(polycycloalkyl)oxy- and -aminophenyl]heterocyclic calcium  
 independent c-AMP phosphodiesterase inhibitor antidepressants)  
 RN 115898-01-6 HCAPLUS  
 CN Benzeneacetonitrile, 3-(bicyclo[2.2.1]hept-2-yloxy)-.alpha.-formyl-4-  
 methoxy- (9CI) (CA INDEX NAME)



L28 ANSWER 15 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:708473 HCAPLUS  
 DN 123:83209  
 ED Entered STN: 29 Jul 1995  
 TI Anti-estrogenic compounds and compositions  
 IN Labrie, Fernand; Merand, Yves  
 PA Endorecherche Inc., Can.  
 SO U.S., 72 pp. Cont.-in-part of U.S. Ser. No. 265,150, abandoned.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC ICM A61K031-445  
 ICS A61K031-44; A61K031-545; C07D401-00  
 NCL 514320000  
 CC 27 14 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 2, 32

FAN.CNT 8

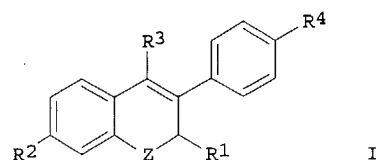
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5395842	A	19950307	US 1991-801704	19911202 <--
HU 52114	A2	19900628	HU 1989-5469	19891027 <--
HU 208150	B	19930830		
JP 2000256390	A2	20000919	JP 2000-62592	19891031 <--
US 5393785	A	19950228	US 1992-913746	19920714 <--
WO 9310741	A2	19930610	WO 1992-CA518	19921201 <--
WO 9310741	A3	19940203		
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, NZ, PL, PT, RO, RU, SD				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9229393	A1	19930628	AU 1992-29393	19921201 <--
AU 681338	B2	19970828		
ZA 9209309	A	19940601	ZA 1992-9309	19921201 <--
EP 615448	A1	19940921	EP 1992-923641	19921201 <--
EP 615448	B1	20020502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
RU 2142945	C1	19991220	RU 1994-31127	19921201 <--
IL 103941	A1	20000726	IL 1992-103941	19921201 <--
JP 2002060384	A2	20020226	JP 2001-207820	19921201 <--
AT 216880	E	20020515	AT 1992-923641	19921201 <--
ES 2176190	T3	20021201	ES 1992-923641	19921201 <--
US 5631249	A	19970520	US 1993-17045	19930212 <--
NO 9402027	A	19940704	NO 1994-2027	19940601 <--
FI 9402568	A	19940727	FI 1994-2568	19940601 <--
US 5840735	A	19981124	US 1994-285354	19940803 <--
US 6060503	A	20000509	US 1995-388207	19950221 <--
US 5686437	A	19971111	US 1995-475710	19950607 <--
US 5686465	A	19971111	US 1995-485739	19950607 <--
AU 9746772	A1	19980219	AU 1997-46772	19971128 <--
JP 10273479	A2	19981013	JP 1998-10654	19980122 <--
JP 3273010	B2	20020408		
AU 760232	B2	20030508	AU 2000-20637	20000303 <--

AU 762751	B2	20030703	AU 2000-34056	20000512 <--
AU 2000034056	A5	20000720		
PRAI US 1988-265150	B2	19881031	<--	
US 1989-377010	B2	19890707	<--	
US 1988-265716	A	19881101	<--	
US 1989-322154	A	19890310	<--	
JP 1989-286010	A3	19891031	<--	
US 1991-801704	A	19911202	<--	
US 1992-917915	A3	19920719	<--	
JP 1993-509666	A3	19921201	<--	
JP 1998-10654	A3	19921201	<--	
WO 1992-CA518	A	19921201	<--	
US 1993-17045	A3	19930212	<--	
US 1994-285354	A2	19940803	<--	
AU 1996-46606	A3	19960220	<--	
AU 1997-46772	A3	19971128	<--	

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	NCL	514320000
US 5395842	ECLA	A61K031/10; A61K031/135; A61K031/165; A61K031/35; A61K031/38; A61K031/40; A61K031/445; A61K031/47; C07C217/18; C07C235/34; C07C317/18; C07D215/14; C07D217/16; C07D235/18; C07D295/0A3; C07D295/08B1D8B; C07D295/18B1D; C07D311/60; C07D335/06A; C07J001/00B2; C07J001/00B4B; C07J001/0B4B1; C07J001/00C5B; C07J001/00C5; C07J001/00C1; C07J001/00C2; C07J001/00C4B; C07J001/00C4B1; C07J001/00CC2; C07J017/00; C07J021/00C1; C07J021/00C2; C07J041/00C40; C07J041/00C70; C07J051/00; C07J053/00C1D; C07J071/00B1; C07J071/00B1C <--
US 5631249	ECLA	A61K031/10; A61K031/135; A61K031/138; A61K031/165; A61K031/352; A61K031/382; A61K031/40; A61K031/40P5; A61K031/4535; A61K031/47; A61K031/47J; A61K031/4709; A61K031/4725; A61K031/575; A61K031/58; A61K031/585; C07C235/34; C07D235/18; C07J001/00B5C2; C07J001/00B5C1; C07J001/00B4B1; C07J001/00B4B; C07J001/00B2; C07J001/00C5C2; C07J001/00C5; C07J001/00C4B1; C07J001/00C4B; C07J001/00C2; C07J001/00C1; C07J017/00; C07J021/00C2; C07J021/00C1; C07J041/00C3; C07J041/00C4D; C07J041/00C40; C07J041/00C60; C07J041/00C70; C07J051/00; C07J053/00C1D; C07J071/00B1; A61K031/4025; A61K031/453 <--
US 5686437	ECLA	A61K031/10; C07J041/00C40; C07J041/00C60; C07J041/00C70; C07J051/00; C07J053/00C1D; C07J071/00B1C; C07J071/00B1; A61K031/135; A61K031/138; A61K031/165; A61K031/352; A61K031/382; A61K031/40; A61K031/40P5; A61K031/4025; A61K031/453; A61K031/4535; A61K031/47; A61K031/47J; A61K031/4709; A61K031/4725; A61K031/575; A61K031/58; A61K031/585; C07C235/34; C07D235/18; C07J001/00B5C2; C07J001/00B5C1; C07J001/00B2; C07J001/00B4B; C07J001/00B4B1; C07J001/00C5; C07J001/00C1; C07J001/00C2; C07J001/00C4B; C07J001/00C4B1; C07J001/00C5C2; C07J017/00; C07J021/00C1; C07J021/00C2; C07J041/00C3; C07J041/00C4D <--

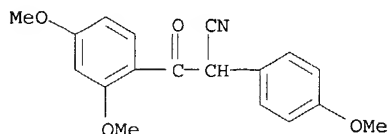
OS MARPAT 123:83209  
GI



AB Title compds. I [Z = alkylene, haloalkylene, oxaalkylene, thiaalkylene, azaalkylene; R1 = substituted phenylene; R2, R4 = H, OH, protected OH; R3 = H, aliphatic] and their 3,4-dihydro derivs. and pharmaceutical compns. containing them were prepared Such pharmaceutical compns. are useful for the

treatment of breast cancer or other diseases whose progress is aided by activation of sex steroid receptors. Thus, I [Z = O, R1 = 4-(2-piperidinoethoxy)phenyl, R2, R4 = OH, R3 = Me, II] was prepared from 2,4-(MeO)2C6H3COCl in 9 steps. II had an ED50 for inhibition of ZR-75-1 cells of 2.55X10<sup>-10</sup> M.

- ST diarylbenzopyranol prepn antiestrogenic; neoplasm inhibitor  
IT diarylbenzopyranol; benzopyranol diaryl prepn antiestrogenic  
IT Neoplasm inhibitors  
(preparation of antiestrogenic diarylbenzopyrans and related compds.)  
IT Estrogens  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(antiestrogens, preparation of antiestrogenic diarylbenzopyrans and related compds.)  
IT 131811-94-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(9repn. of antiestrogenic diarylbenzopyrans and related compds.)  
IT 131811-54-6P 134227-19-3P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of antiestrogenic diarylbenzopyrans and related compds.)  
IT 104-47-2, 4-Methoxyphenylacetonitrile 123-08-0 434-22-0, 19-Nortestosterone 1440-60-4, N-Chloroacetyl piperidine 1611-56-9, 11-Bromo-1-undecanol 2008-75-5, 1-(2-Chloroethyl)piperidine hydrochloride 2398-37-0, 3-Bromoanisole 2472-22-2 3143-02-0 3589-92-2 3647-69-6, 4-(2-Chloroethyl)morpholine hydrochloride 4390-94-7 39096-59-8 39828-35-8, 2,4-Dimethoxybenzoyl chloride 52056-69-6 103483-33-6 151533-59-4 151533-66-3 151533-68-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of antiestrogenic diarylbenzopyrans and related compds.)  
IT 2150-41-6P, Methyl 2,4-dimethoxybenzoate 2590-41-2P 4999-76-2P 17720-60-4P 39604-64-3P 55592-08-0P 55592-09-1P 55592-10-4P 55592-11-5P 67804-60-8P 98008-56-1P 98013-89-9P 127947-01-7P 127947-02-8P 130064-21-0P 130064-26-5P 130064-27-6P 131811-57-9P 131811-59-1P 131811-61-5P 131811-71-7P 131811-72-8P 131811-73-9P 131811-74-0P 131811-75-1P 131811-76-2P 131811-77-3P 131811-78-4P 131811-79-5P 131811-80-8P 131811-81-9P 131811-82-0P 131811-83-1P 131811-84-2P 131811-85-3P 131811-86-4P 131811-87-5P 131811-88-6P 131811-89-7P 131811-90-0P 131811-91-1P 131811-92-2P 131811-93-3P 131811-95-5P 131811-96-6P 131838-68-1P 132593-12-5P 151533-32-3P 151533-33-4P 151533-35-6P 151533-39-0P 151533-44-7P 151533-45-8P 151533-46-9P 151533-52-7P 151533-55-0P 151533-57-2P 151533-61-8P 151533-64-1P 151533-67-4P 165535-11-5P 165535-12-6P 165535-13-7P 165535-14-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of antiestrogenic diarylbenzopyrans and related compds.)  
IT 131811-52-4P 131811-53-5P 131811-55-7P 131811-56-8P 131811-58-0P 131811-60-4P 131811-64-8P 131811-65-9P 131811-66-0P 131811-70-6P 151533-34-5P 151533-50-5P 151533-53-8P 151533-56-1P 151533-58-3P 151533-62-9P 151533-65-2P 151533-72-1P 151533-76-5P 151533-77-6P 165535-15-9P  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of antiestrogenic diarylbenzopyrans and related compds.)  
IT 132593-12-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of antiestrogenic diarylbenzopyrans and related compds.)  
RN 132593-12-5 HCAPLUS  
CN Benzenepropanenitrile, 2,4-dimethoxy-.alpha.-(4-methoxyphenyl)-.beta.-oxo- (9CI) (CA INDEX NAME)





PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
PI	US 5234946	A	19930810	US 1991-753611	19910830 <--
	ZA 8808792	A	19890830	ZA 1988-8792	19881124 <--
	JP 03193746	A2	19910823	JP 1988-296840	19881124 <--
	CN 1037141	A	19891115	CN 1988-109274	19881126 <--
	ZA 8908464	A	19910130	ZA 1989-8464	19891107 <--
PRAI	JP 1987-299584		19871127	<--	
	JP 1988-96286		19880419	<--	
	JP 1988-113310		19880510	<--	
	JP 1988-285381		19881111	<--	
	US 1988-274972		19881122	<--	
	US 1990-465209		19900308	<--	
	US 1990-533532		19900605	<--	

CLASS		
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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US 5234946	ICM	A61K031-38
	ICS	C07D333-32
	NCL	514444000

CCN(CC)Cc1ccc(Oc2cc3sc(cc3s2)-c4cc5sc(cc5s4)S)cc1/C=C/C#CC(C)(C)C

Searched by Noble Jarrell

155293-43-9P 155293-44-0P 155293-45-1P 155293-46-2P 155293-47-3P  
 155293-48-4P 155293-49-5P 155293-50-8P 155293-51-9P 155293-52-0P  
**155293-53-1P** 155293-54-2P 155293-55-3P 155293-56-4P  
 155293-57-5P 155293-58-6P 155293-59-7P 155293-60-0P 155293-61-1P  
 155293-62-2P 155293-63-3P 155293-64-4P 155293-65-5P 155293-66-6P  
 155293-67-7P 155293-68-8P 155293-69-9P 155293-70-2P 155293-71-3P  
 155293-72-4P 155293-73-5P 155293-74-6P 155293-75-7P 155293-76-8P  
 155293-77-9P 155293-78-0P 155293-79-1P 155293-80-4P 155293-81-5P  
 155293-82-6P 155293-83-7P 155293-84-8P 155293-85-9P 155293-86-0P  
 155293-87-1P 155293-88-2P 155293-89-3P 155293-90-6P 155293-91-7P  
 155293-92-8P 155293-93-9P 155293-94-0P 155293-95-1P 155293-96-2P  
 155293-97-3P 155293-98-4P 155293-99-5P 155294-00-1P 155294-01-2P  
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 155294-07-8P 155294-08-9P 155294-09-0P 155294-10-3P 155294-11-4P  
 155294-12-5P 155294-13-6P 155294-14-7P 155294-15-8P 155294-16-9P  
 155294-17-0P 155294-18-1P 155294-19-2P 155294-20-5P 155294-21-6P  
 155294-22-7P 155294-23-8P 155294-24-9P 155294-25-0P 155294-26-1P  
 155294-27-2P 155294-28-3P 155294-29-4P 155294-30-7P 155294-31-8P  
 155294-32-9P 155294-33-0P 155294-34-1P 155294-35-2P 155294-36-3P  
 155294-37-4P 155294-38-5P 155294-39-6P 155294-40-9P 155294-41-0P  
 155294-42-1P 155294-43-2P 155294-44-3P 155294-45-4P 155294-46-5P  
 155294-47-6P 155294-48-7P 155294-49-8P 155294-50-1P 155294-51-2P  
 155294-52-3P 155294-53-4P 155294-54-5P 155294-55-6P 155294-56-7P  
 155294-57-8P 155294-58-9P 155294-59-0P 155294-60-3P 155294-61-4P  
 155294-62-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as antiarteriosclerotic, anticholesteremic or hypolipemic)

IT 78629-21-7P 123926-61-4P 129746-42-5P, 3-(3-Thienyl)benzaldehyde  
 129746-44-7P 129747-36-0P 129747-37-1P 129747-72-4P 136719-34-1P  
 155294-74-9P 155294-75-0P 155294-76-1P 155294-77-2P 155294-78-3P  
 155294-79-4P 155294-80-7P 155294-81-8P 155294-82-9P,  
 [2,3'-Bithiophene]-4-methanol 155294-83-0P 155294-84-1P 155294-85-2P  
 155294-86-3P 155294-87-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for (alkenynyl)benzylamine  
 (anticholesteremic, antiarteriosclerotic))

IT 155294-72-7P 155294-73-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for (alkenynyl)furfurylamine  
 (anticholesteremic, antiarteriosclerotic))

IT 155294-92-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for (alkenynyl)oxazolemethanamine  
 (anticholesteremic, antiarteriosclerotic))

IT 155294-89-6P 155294-90-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for (alkenynyl)thiophenemethanamine  
 (anticholesteremic, antiarteriosclerotic))

IT 1008-74-8, 5-(3-Methylphenyl)isoxazole 4515-89-3, 1-  
 Methylcyclopropanecarboxaldehyde 6138-90-5, Geranyl bromide  
 24033-03-2, 3-Benzoyloxybenzyl chloride 39687-95-1, Methyl  
 isocyanoacetate 67978-51-2 67978-52-3 76100-81-7 89929-93-1,  
 3-(2-Furyl)benzyl alcohol 116939-14-1 123925-85-9 123926-30-7  
 123926-39-6 123926-40-9 123926-41-0 123926-54-5 123926-55-6  
 123926-61-4 129746-41-4 129747-33-7 129747-34-8 129747-39-3  
 129747-59-7 136719-31-8 136719-33-0, [3,3'-Bithiophene]-5-methanol  
 138139-92-1 155294-63-6 155294-64-7 155294-65-8 155294-66-9  
 155294-67-0 155294-68-1 155294-69-2 155294-70-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for (alkenynyl)benzylamine (anticholesteremic,  
 antiarteriosclerotic))

IT 89929-85-1, 3-(3-Thienyl)benzyl bromide 129777-47-5 155294-71-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for (alkenynyl)furfurylamine (anticholesteremic,  
 antiarteriosclerotic))

IT 155294-93-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for (alkenynyl)isoxazolemethanamine (anticholesteremic,  
 antiarteriosclerotic))

IT 155294-91-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for (alkenynyl)oxazolemethanamine (anticholesteremic,  
 antiarteriosclerotic))

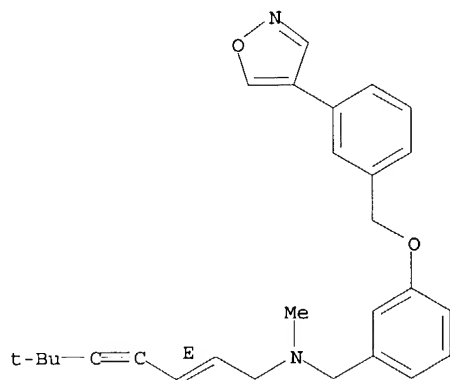
IT 155294-88-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for (alkenynyl)thiophenemethanamine (anticholesteremic,

antiarteriosclerotic))  
 IT 132052-93-8, Epoxidase  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (squalane epoxidase inhibitors, (alkenynyl)benzylamines and analogs)  
 IT 155293-53-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as antiarteriosclerotic, anticholesteremic or hypolipemic)  
 RN 155293-53-1 HCAPLUS  
 CN Benzenemethanamine, N-(6,6-dimethyl-2-hepten-4-ynyl)-3-[[3-(4-isoxazolyl)phenyl]methoxy]-N-methyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



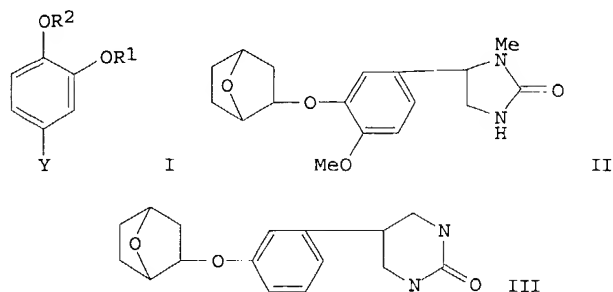
L28 ANSWER 17 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1993:101978 HCAPLUS  
 DN 118:101978  
 ED Entered STN: 19 Mar 1993  
 TI Preparation of aryl substituted nitrogen heterocyclic antidepressants  
 IN Saccomano, Nicholas A.; Vinick, Fredric J.  
 PA Pfizer Inc., USA  
 SO U.S., 28 pp. Division of U.S. Ser. No. 155,932.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07D233-30  
 ICS A61K031-415  
 NCL 514392000  
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5128358	A	19920707	US 1991-696690	19910530 <--
	US 5459145	A	19951017	US 1988-155932	19880119 <--
	US 5196426	A	19930323	US 1992-854136	19920319 <--
	US 5294730	A	19940315	US 1992-984190	19921120 <--
	US 5414127	A	19950509	US 1994-184092	19940119 <--
PRAI	US 1988-155932	A3	19880119	<--	
	US 1991-696690	A3	19910830	<--	
	US 1992-854136	A3	19920319	<--	
	US 1992-984190	A3	19921120	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5128358	ICM	C07D233-30
	ICS	A61K031-415
	NCL	514392000
US 5459145	ECLA	C07C217/60; C07C255/37; C07D233/32; C07D233/42; C07D233/78; C07D239/10B; C07D239/22D1; C07D029/36B; C07D285/08B; C07D285/10B; C07D487/04; C07D487/04 <--

OS MARPAT 118:101978  
 GI



AB Title compds. I (R1 = C7-11 bi-, tricycloalkyl, indan-2-yl; R2 = Me, Et; Y = (substituted) (saturated) 5-6-membered N-containing heterocyclyl), salt, optical isomers, diastereomers, useful as antidepressants (no data), are prepared A mixture of endo- and exo-.alpha.-(methylamino)-3-bicyclo[2.2.1]hept-2-yloxy)-4-methoxybenzeneacetonitrile (preparation given) in THF were treated with 1,1-carbonyldiimidazole, the reaction stirred for 24 h at room temperature, and treated with NaOH, HCl, H2O and saturated salt solution to give endo- and exo-title compound II. Similarly prepared was endo- and exo-title compound III. Addnl. I were prepared

ST aryl heterocycle prepn antidepressant; imidazolidinone polyalkyloxyphenyl prepn antidepressant; thiadiazolidinone bicycloheptyloxyphenyl prepn antidepressant; pyrimidinone bicycloheptyloxyphenyl prepn antidepressant; pyrazole bicycloheptyloxyphenyl prepn antidepressant; imidazopyrimidine bicycloheptyloxyphenyl prepn antidepressant; pyrazolopyrimidine bicycloheptyloxyphenyl prepn antidepressant

IT Antidepressants

(aryl nitrogen heterocycles)

IT 1702-10-9P 10271-43-9P 18684-63-4P, Bicyclo[2.2.2]octan-2-ol  
 115897-62-6P 115897-63-7P 115897-65-9P 115897-66-0P 115897-69-3P  
 115897-78-4P 115897-79-5P 115897-81-9P 115897-82-0P 115897-85-3P  
 115897-86-4P 115897-88-6P 115897-89-7P 115897-91-1P 115897-92-2P  
 115897-94-4P 115897-95-5P 115897-99-9P 115898-02-7P  
 115898-03-8P 115898-04-9P 115898-05-0P 115898-09-4P 115898-10-7P  
 115898-16-3P 115898-17-4P 115898-18-5P 115898-20-9P 115898-21-0P  
 115898-37-8P 115898-38-9P 115898-39-0P 115898-42-5P 115898-51-6P  
 115898-52-7P 115898-54-9P 115898-55-0P 115898-57-2P 115898-58-3P  
 115898-59-4P 115898-62-9P 115898-63-0P 115898-64-1P 115898-65-2P  
 115898-66-3P 115898-67-4P 115898-68-5P 115898-69-6P 115898-70-9P  
 115898-73-2P 115898-74-3P 115898-75-4P 115898-76-5P 115898-77-6P  
 115898-78-7P 115898-79-8P 131408-40-7P 141184-64-7P 144033-83-0P  
 144033-84-1P 144033-85-2P 144033-86-3P 144033-87-4P 144033-92-1P  
 144033-93-2P 144034-08-2P 144034-09-3P 144034-10-6P 144034-11-7P  
 144034-12-8P 144034-13-9P 144034-14-0P 144034-15-1P 144034-16-2P  
 144034-17-3P 144034-18-4P 144034-20-8P 144124-74-3P  
 144365-77-5P 144365-78-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of antidepressants)

IT 115897-70-6P 115897-71-7P 115897-73-9P 115897-75-1P 115897-77-3P  
 115897-80-8P 115897-83-1P 115897-84-2P 115897-87-5P 115897-90-0P  
 115897-93-3P 115897-96-6P 115897-97-7P 115897-98-8P 115898-00-5P  
 115898-06-1P 115898-07-2P 115898-08-3P 115898-11-8P 115898-12-9P  
 115898-19-6P 115898-22-1P 115898-29-8P 115898-30-1P 115898-34-5P  
 115898-36-7P 115919-88-5P 144033-88-5P 144033-89-6P 144033-90-9P  
 144033-91-0P 144033-94-3P 144033-95-4P 144033-96-5P 144033-97-6P  
 144033-98-7P 144033-99-8P 144034-00-4P 144034-01-5P 144034-02-6P  
 144034-03-7P 144034-04-8P 144034-05-9P 144034-06-0P 144034-07-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, antidepressant)

IT 57-13-6, Urea, reactions 64-04-0, Benzeneethanamine 105-53-3, Diethyl malonate 107-11-9, 2-Propen-1-amine 120-80-9, Pyrocatechol, reactions 124-63-0, Methanesulfonyl chloride 302-01-2, Hydrazine, reactions 372-09-8, Cyanoacetic acid 497-36-9 497-38-1, Norcamphor 530-62-1 542-69-8 557-66-4, Ethylaminehydrochloride 621-59-0, Isovanillin 700-57-2, 2-Adamantanol 931-64-6, Bicyclo[2.2.2]oct-2-ene 1820-80-0, 1H-Pyrazol-3-amine 1965-38-4 2534-77-2, exo-2-Bromonorbornane 6160-65-2 6351-10-6, 1-Indanol 7374-90-5 7803-58-9, Sulfamide 13380-89-7 13380-94-4 42383-61-9, 2-Aminoimidazolesulfate 50447-20-6 144034-19-5

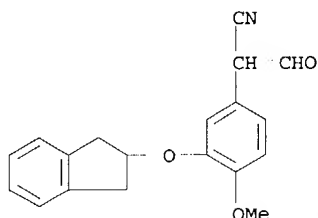
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in preparation of heterocyclic antidepressants)

IT 115898-02-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in preparation of antidepressants)

RN 115898-02-7 HCAPLUS

CN Benzeneacetonitrile, 3-[(2,3-dihydro-1H-inden-2-yl)oxy]-.alpha.-formyl-4-methoxy- (9CI) (CA INDEX NAME)



L28 ANSWER 18 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:61950 HCAPLUS

DN 114:61950

ED Entered STN: 23 Feb 1991

TI Preparation and formulation of tetra- and decahydroquinoline-4-carboxylic acids and analogs for use in tissue irrigating solutions

IN Leclerc, Gerard; Ruhland, Beatrice; Andermann, Guy; De Burlet, Georges; Dietz, Michel

PA Laboratoires Alcon S. A., Fr.

SO U.S., 16 pp.

CODEN: USXXAM

DT Patent

LA English

IC ICM C07D215-48

ICS A61K031-47

NCL 514311000

CC 27-17 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4952573	A	19900828	US 1988-172047	19880323 <--
PRAI	US 1988-172047		19880323 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4952573	ICM	C07D215-48
	ICS	A61K031-47
	NCL	514311000

OS CASREACT 114:61950

AB The title compds. having .gamma.-aminobutyric acid (GABA) like activity, were prepared for use in tissue irrigating solns. to promote corneal deswelling during otic surgery. Thus, N-methylquinoline-4-carboxamide was stirred with Ni-Al alloy in aqueous MeOH containing KOH and the product refluxed 14 h with aqueous HCl to give 1,2,3,4-tetrahydroquinoline-4-carboxylic acid-HCl, which gave 34.6 .mu.m reduction of bovine corneal swelling after 3 h perfusion at 0.01 mM compared to 17.2 .mu.m reduction by GABA under the same conditions.

ST quinolinecarboxylate prepn otic tissue irrigant

IT Edema

(corneal, surgery associated, isoquinolinecarboxylates and analogs for prevention of)

IT Eye, disease or disorder

(cornea, surgery associated edema of, quinolinecarboxylates and analogs for prevention of)

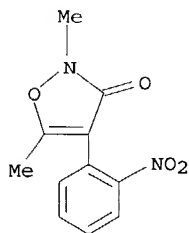
IT Pharmaceutical dosage forms

(solns., ophthalmic, irrigation, quinolinecarboxylates and analogs for prevention of surgery-associated corneal edema)

IT 123705-23-7P

RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in preparation of otic tissue irrigant)

IT 108890-73-9P 123705-20-4P 123705-21-5P 123705-22-6P  
 123705-24-8P 123705-25-9P 123705-26-0P  
 123705-27-1P 123705-28-2P 131753-21-4P 131753-24-7P  
 131753-25-8P 131753-26-9P 131753-27-0P 131753-29-2P  
 131753-30-5P 131753-31-6P 131753-33-8P 131753-34-9P 131753-35-0P  
 131753-36-1P 131753-37-2P 131753-39-4P 131753-40-7P  
 131774-41-9P 131774-42-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, in preparation of otic tissue irrigant)  
 IT 13337-72-9P 13337-80-9P 131753-22-5P 131753-23-6P 131753-28-1P  
 131753-32-7P 131753-38-3P 131753-41-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as otic tissue irrigant)  
 IT 87-25-2 486-74-8, 4-Quinolinecarboxylic acid 541-41-3,  
 Ethylchloroformate 2969-81-5 10565-19-2 72802-70-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, in preparation of otic tissue irrigant)  
 IT 123705-23-7P  
 RL: SPN (Synthetic preparation); SPN (Synthetic  
 preparation); PREP (Preparation)  
 (formation of, in preparation of otic tissue irrigant)  
 RN 123705-23-7 HCAPLUS  
 CN 3(2H)-Isoxazolone, 2,5-dimethyl-4-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



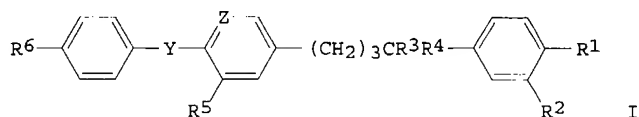
L28 ANSWER 19 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1989:57524 HCAPLUS  
 DN 110:57524  
 ED Entered STN: 17 Feb 1989  
 TI Preparation of 6-pyridyl- and 6-phenyl-3-phenyl-1-hexenes and -1-hexynes  
 as insecticides and acaricides  
 IN Matsuo, Noritada; Tsushima, Kazunori; Nishida, Sumio; Yano, Toshihiko;  
 Hirano, Masachika  
 PA Sumitomo Chemical Co., Ltd., Japan  
 SO U.S., 23 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A01N043-40  
 ICS A01N033-10; C07D405-10; C07C149-31  
 NCL 514717000  
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 5  
 FAN.CNT 1  

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4772633	A	19880920	US 1986-831180	19860220 <--
PRAI US 1986-831180		19860220 <--		

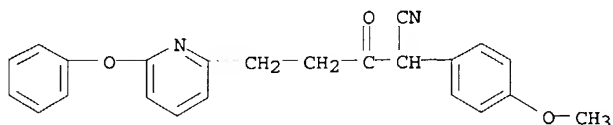
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4772633	ICM	A01N043-40
	ICS	A01N033-10; C07D405-10; C07C149-31
	NCL	514717000

OS CASREACT 110:57524; MARPAT 110:57524  
 GI



- AB The title compds. (I; R1, R2 = H, halo, alkyl, CF3, alkoxy, alkenyloxy, haloalkoxy; R1R2 = OCH2O; R3 = CH:CH, C.tplbond.C; R4 = H, alkyl; R5 = H, F; R6 = H, halo, alkyl, alkoxy, CF3; Y = O, S, CH2, NH; Z = N, CH) were prepared 4-(EtO)C6H4CH2CN was stirred 1 h at -50.degree. with (Me2CH)2NLi in THF whereupon MeI was added and stirring continued 13 h to give 4-(EtO)C6H4CHMeCN which was stirred 30 min with NaH in DMF, 3-(PhO)C6H4(CH2)3Br added, and stirring continued 12 h to give 3-(PhO)C6H4(CH2)3CMe(CN)C6H4(OEt)-4. The latter was reduced with Dibal in PhMe to the corresponding aldehyde which was added to Ph3PMeBr in THF previously stirred with BuLi and the mixture stirred 14 h to give 3-(PhO)C6H4(CH2)3CMe(CH:CH2)C6H4(OEt)-4 which caused .gtoreq.90% mortality to Culex pipiens pallens larvae at 3.5 ppm in aqueous solution
- ST pyridylphenylhexene hexyne prepn insecticide acaricide; hexene hexyne diphenyl prepn insecticide acaricide
- IT Acaricides  
Insecticides  
(pyridylphenyl- and diphenylhexenes and -hexynes)
- IT 51558-05-5P, 2-(4-Ethoxyphenyl)propionitrile 105128-01-6P 105128-02-7P  
105128-03-8P 105128-04-9P 105128-05-0P 105128-06-1P  
105128-07-2P 105128-08-3P 105128-09-4P 105128-10-7P 105128-14-1P  
105128-15-2P 118365-86-9P 118365-87-0P 118365-88-1P 118365-89-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in preparation of insecticides and acaricides)
- IT 105127-61-5P 105127-62-6P 105127-63-7P 105127-64-8P 105127-65-9P  
105127-66-0P 105127-67-1P 105127-68-2P 105127-69-3P 105127-70-6P  
105127-71-7P 105127-72-8P 105127-73-9P 105127-74-0P 105127-75-1P  
105127-76-2P 105127-77-3P 105127-78-4P 105127-79-5P 105127-80-8P  
105127-81-9P 105127-82-0P 105127-83-1P 105127-84-2P 105127-85-3P  
105127-86-4P 105127-87-5P 105127-88-6P 105127-89-7P 105127-90-0P  
105127-91-1P 105127-92-2P 105127-93-3P 105127-94-4P 105127-95-5P  
105127-97-7P 105127-98-8P 105127-99-9P 105147-96-4P 105147-97-5P  
105147-98-6P 105147-99-7P 118383-67-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as insecticide and acaricide)
- IT 104-47-2, 4-Methoxyphenylacetonitrile  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in preparation of insecticides and acaricides)
- IT 5927-18-4, Trimethylphosphonoacetate 6775-77-5, 4-Ethoxyphenylacetonitrile 68523-22-8, 2-Formyl-6-phenoxy pyridine  
105128-00-5, 3-(3-Phenoxyphenyl)propylbromide 105128-13-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in preparation of insecticides and acaricides)
- IT 105128-06-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in preparation of insecticides and acaricides)
- RN 105128-06-1 HCAPLUS
- CN 2-Pyridinepentanenitrile, .alpha.-(4-methoxyphenyl)-.beta.-oxo-6-phenoxy-(9CI) (CA INDEX NAME)



L28 ANSWER 20 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1987:63041 HCAPLUS  
DN 106:63041  
ED Entered STN: 07 Mar 1987  
TI Synergistic insecticidal compositions containing dione esters  
IN Sousa, Anthony A.

PA Union Carbide Corp., USA  
 SO U.S., 17 pp. Cont. of U.S. Ser. No. 277,731, abandoned.  
 CODEN: USXXAM

DT Patent

LA English

IC ICM A01N037-34

ICS A01N053-00

NCL 514521000

CC 5-4 (Agrochemical Bioregulators)

Section cross-reference(s): 25

FAN.CNT 1

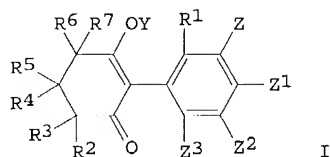
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4613617	A	19860923	US 1985-724960	19850423 <--
PRAI	US 1981-277731		19810626	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4613617	ICM	A01N037-34
	ICS	A01N053-00
	NCL	514521000

OS CASREACT 106:63041

GI



I

AB Dione ester derivs. I [Z, Z1, Z2, Z3 = H, haloalkyl, polyhaloalkyl, halo, alkyl, alkoxy, cyano, NO2, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, CONH2, NH2; Y = COR; R = H, halo, (un)substituted alkyl, alkenyl, alkynyl, bicycloalkyl, bicycloalkenyl, cycloalkyl, cycloalkenyl, Ph, phenylalkyl, naphthyl, naphthylalkyl; R1 = alkyl, polyhaloalkyl, haloalkyl, halo; R2, R3, R4, R5, R6, R7 = H, (un)substituted alkyl, Ph, cyano, halo, NO2, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, dialkylamino, etc.] are prepared as insecticides. I are synergistic with known insecticides. Thus, 2.0 g 2-ethylhexanoyl chloride was added to a solution of 1.50 g 2-(2',4'-dimethylphenyl)-5,5-dimethyl-1,3-cyclohexanedione and 1.94 g pyridine in 10 mL CHCl3. The mixture was stirred for 2 h at room temperature, then refluxed for 12 h to give 1.15 g 3-(2-ethylhexanoyloxy)-5,5-dimethyl-2-(2',4'-dimethylphenyl)-2-cyclohexenone (II). II and carbaryl synergistically kill the housefly (*Musca domestica*).

ST cyclohexenone prepn synergistic insecticide

IT Insecticides

(synergistic, phenylcyclohexenone-containing compns.)

IT 108-67-8, Mesitylene, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation of, with diazocyclohexanedione)

IT 126-81-8, 5,5-Dimethyl-1,3-cyclohexanedione

RL: BIOL (Biological study)

(condensation of, with dichloronitrobenzene)

IT 99-54-7, 3,4-Dichloronitrobenzene 20098-48-0, 3,4,5-Trichloronitrobenzene

RL: BIOL (Biological study)

(condensation of, with dimethylcyclohexanedione)

IT 1460-08-8, 2-Diazocyclohexane-1,3-dione

RL: BIOL (Biological study)

(condensation of, with mesitylene)

IT 1807-68-7, 2-Diazo-5,5-dimethylcyclohexane-1,3-dione

RL: BIOL (Biological study)

(condensation of, with xylene)

IT 68427-57-6 68429-54-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclocondensation of)

IT 760-67-8, 2-Ethylhexanoyl chloride

RL: BIOL (Biological study)

(esterification with (chlorophenyl)dimethylcyclohexanedione)

IT 142-61-0, Hexanoyl chloride

RL: BIOL (Biological study)

Searched by Noble Jarrell



(esterification with (dimethylphenyl)dimethylcyclohexanedione)

IT 298-00-0, Methyl parathion 35400-43-2, Sulprofos 51630-58-1  
52645-53-1, Permethrin 52918-63-5, Decamethrin  
RL: BIOL (Biological study)  
(insecticidal composition containing, synergized by dione ester)

IT 108-88-3, Toluene, biological studies  
RL: BIOL (Biological study)  
(photoreaction of, with diazodecalindione)

IT 98-19-1  
RL: BIOL (Biological study)  
(photoreaction of, with diazodimethylcyclohexanedione)

IT 68427-55-4P 68427-57-6P 68427-58-7P 68427-60-1P  
68427-62-3P 68427-63-4P 101582-73-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation of)

IT 68427-39-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and deamination of)

IT 68427-40-7P 68427-41-8P 68427-43-0P 68427-44-1P 68427-45-2P  
68427-46-3P 68427-47-4P 68427-49-6P 68427-50-9P 68427-52-1P  
68427-56-5P 68427-59-8P 68427-61-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and esterification of)

IT 68427-51-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and photoreaction of, with toluene)

IT 68427-48-5P, 2-Diazo-5-phenylcyclohexane-1,3-dione  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reaction of, with mesitylene)

IT 68427-38-3P 68427-42-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reduction of)

IT 68427-64-5P 68427-65-6P 68427-67-8P 68427-68-9P 68427-69-0P  
68428-15-9P 72619-67-1P 83786-58-7P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except  
adverse); BSU (Biological study, unclassified); SPN (Synthetic  
preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as insecticide)

IT 16213-85-7 68429-53-8, 2,4-Dimethylbenzylcyanide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with di-Et dimethylglutarate)

IT 108-38-3, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diazocyclohexanedione derivative, in synthesis of  
insecticides)

IT 17804-59-0, Diethyl 3,3-dimethylglutarate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with dimethylbenzyl cyanide)

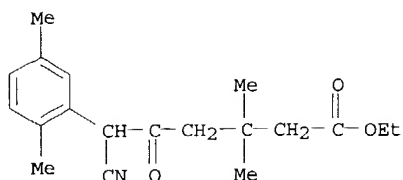
IT 941-55-9, Tosyl azide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylcyclohexanedione)

IT 493-72-1, 5-Phenylcyclohexane-1,3-dione 68429-52-7, Decalin-1,3-dione  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with tosyl azide)

IT 68427-60-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation of)

RN 68427-60-1 HCAPLUS

CN Benzenehexanoic acid, .epsilon.-cyano-.beta.,.beta.,2,5-tetramethyl-  
.delta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



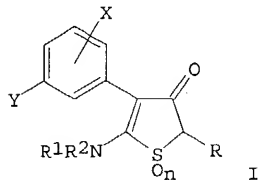
L28 ANSWER 21 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1986:552917 HCAPLUS  
 DN 105:152917  
 ED Entered STN: 01 Nov 1986  
 TI Herbicidal 5-amino-3-oxo-4-(substituted phenyl)-2,3-dihydrothiophenes and their derivatives  
 IN Ward, Carl E.  
 PA Chevron Research Co. , USA  
 SO U.S., 22 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A01N043-02  
 ICS A01N043-40; A01N043-36; C07D333-16  
 NCL 071090000  
 CC 27-8 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 5  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4596595	A	19860624	US 1984-623805	19840622 <--
WO 8702220	A1	19870423	WO 1985-US2004	19851011 <--
W: AT, AU, BR, CH, DE, GB, JP, KR, NL				
AU 8548672	A1	19870505	AU 1985-48672	19851011 <--
AU 593224	B2	19900208		
NL 8520343	A	19870901	NL 1985-20343	19851011 <--
BR 8507300	A	19871103	BR 1985-7300	19851011 <--
DE 3590848	T	19871210	DE 1985-3590848	19851011 <--
JP 63501073	T2	19880421	JP 1985-504754	19851011 <--
CH 673651	A	19900330	CH 1987-2274	19851011 <--
AT 8509085	A	19930115	AT 1985-90	19851011 <--
AT 396470	B	19930927		
CA 1280752	A1	19910226	CA 1985-493921	19851025 <--
IL 76882	A1	19920329	IL 1985-76882	19851030 <--
FR 2590253	A1	19870522	FR 1985-17064	19851119 <--
FR 2590253	B1	19880212		
GB 2191191	A1	19871209	GB 1987-9948	19870427 <--
GB 2191191	B2	19890913		
PRAI US 1984-623805		19840622 <--		
WO 1985-US2004		19851011 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4596595	ICM	A01N043-02
	ICS	A01N043-40; A01N043-36; C07D333-16
	NCL	071090000

OS CASREACT 105:152917  
 GI



AB The title compds. [I; R = (halo)alkyl, cycloalkyl, (cycloalkyl)alkyl, (halo)alkenyl, alkoxy, alkylthio, alkoxyalkyl, 4-FC6H4, (un)substituted Ph, naphthyl, indenyl, substituted arylmethyl; R1 = H, C1-4 alkyl; R2 = H,

C1-4 alkyl, C3-4 alkenyl, alkoxy-carbonylalkyl, alkoxyalkyl, alkylthioalkyl; R1R2N = heterocyclyl; X = H, alkyl, alkoxy, halo, CF<sub>3</sub>; Y = alkyl, alkoxy, halo, haloalkyl, haloalkoxy, haloalkylthio; n = 0-2] and their salts, useful as herbicides and plant growth regulators, were prepared. Thus, MeSCH<sub>2</sub>COCH(C<sub>6</sub>H<sub>4</sub>CF<sub>3</sub>-3)CN in THF was treated with (Me<sub>3</sub>Si)<sub>2</sub>NLi and MeI to give MeCH(SMe)COCH(C<sub>6</sub>H<sub>4</sub>CF<sub>3</sub>-3)CN, which was cyclized in AcOH with H<sub>2</sub>SO<sub>4</sub> to give I (R = Me; R<sub>1</sub> = R<sub>2</sub> = X = H; Y = CF<sub>3</sub>; n = 0) (II). In preemergence tests, II at 27.5 .mu.g/cm<sup>2</sup> was 100% phytotoxic to lambsquarter and crab- and watergrass with no damage to wild oats and rice.

ST aminophenylthiophenone prepn herbicide plant growth regulator; thiophenone aminophenyl prepn herbicide

IT Herbicides

(aminophenyldihydrothiophenones and their oxides)

IT Plant hormones and regulators

RL: RCT (Reactant); RACT (Reactant or reagent)

(aminophenyldihydrothiophenones and their oxides)

IT Molecular structure-biological activity relationship

(herbicidal, of aminophenyldihydrothiophenones and their oxides)

IT 101-97-3 104456-12-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation of, with acetonitrile derivative)

IT 2338-76-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation of, with phenylacetates)

IT 104456-10-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(homologation of)

IT 104456-09-9P 104456-11-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, thiophene from)

IT 68084-26-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, with sulfur, thiophene from)

IT 18729-76-5P 18729-77-6P 104456-64-6P 104456-65-7P 104456-66-8P

104456-67-9P 104456-68-0P 104456-69-1P 104456-70-4P 104456-71-5P

104456-72-6P 104456-73-7P 104456-74-8P 104456-75-9P 104456-76-0P

104456-77-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and herbicidal activity of)

IT 104456-08-8P 104456-13-5P 104456-14-6P 104456-15-7P 104456-16-8P

104456-17-9P 104456-18-0P 104456-19-1P 104456-20-4P 104456-21-5P

104456-22-6P 104456-23-7P 104456-24-8P 104456-25-9P 104456-26-0P

104456-27-1P 104456-28-2P 104456-29-3P 104456-30-6P 104456-31-7P

104456-32-8P 104456-33-9P 104456-34-0P 104456-35-1P 104456-36-2P

104456-37-3P 104456-38-4P 104456-39-5P 104456-40-8P 104456-41-9P

104456-42-0P 104456-43-1P 104456-44-2P 104456-45-3P 104456-46-4P

104456-47-5P 104456-48-6P 104456-49-7P 104456-50-0P 104456-51-1P

104456-52-2P 104456-53-3P 104456-54-4P 104456-55-5P 104456-56-6P

104456-57-7P 104456-58-8P 104456-59-9P 104456-60-2P 104456-61-3P

104456-62-4P 104456-63-5P 104456-78-2P 104471-83-2P 104471-84-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as herbicide and plant growth regulator)

IT 104456-09-9P

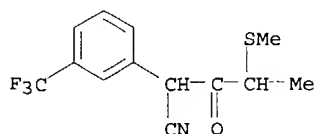
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, thiophene from)

RN 104456-09-9 HCAPLUS

CN Benzeneacetonitrile, .alpha.-[2-(methylthio)-1-oxopropyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 22 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1986:420517 HCAPLUS  
 DN 105:20517  
 ED Entered STN: 26 Jul 1986  
 TI Herbicidal 5-amino-3-oxo-4-(substituted-phenyl)-2,3-dihydrofuran  
 IN Ward, Carl E.  
 PA Chevron Research Co. , USA  
 SO U.S., 14 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM A01N043-08  
 ICS C07D307-66  
 NCL 071088000  
 CC 5-3 (Agrochemical Bioregulators)  
 Section cross-reference(s): 27

FAN.CNT 1

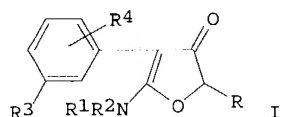
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4568377	A	19860204	US 1985-727459	19850426 <--
PRAI US 1985-727459		19850426 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4568377	ICM	A01N043-08
	ICS	C07D307-66
	NCL	071088000

OS CASREACT 105:20517

GI



AB The title compds. I [R = (un)substituted Ph, naphth-1-yl, inden-1-yl; R2 = H, alkyl; R2 = H, alkyl, alkenyl, alkoxythioalkyl, etc.; NR1R2 = ring; R3 = CN, NO2, alkoxy, carbonyl, etc.; R4 = H, halo, alkyl, alkoxy, F3C] are herbicides. Thus, pre-emergence I (R = Ph, R1 = R4 = H, R2 = Me, R3 = CO2Et) (27.5 .mu.g/cm2) totally controlled lambsquarters, mustard, crabgrass, and other weeds, in pot expts. I are prepared by cyclization of the corresponding acylacetone nitriles.

ST furanone herbicide prepn

IT Herbicides

(aminooxophenyldihydrofurans)

IT 68432-92-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (acylation of)

IT 103-80-0

RL: BIOL (Biological study)  
 (condensation of, with methoxycarbonylphenylacetyl)

IT 101480-90-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (methylation of)

IT 101480-83-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization of)

IT 23145-00-8P 23145-02-0P 76996-63-9P 96541-91-2P 96541-92-3P

96541-93-4P 96541-94-5P 96541-95-6P 96541-96-7P 96541-97-8P

96572-49-5P 96572-50-8P 96572-51-9P 96906-18-2P 96906-20-6P

96906-21-7P 101480-84-6P 101480-85-7P 101480-88-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of, as herbicide)

IT 101480-86-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, with herbicide)

IT 106-95-6, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

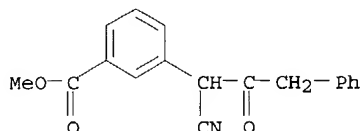
(reaction of, with (fluorophenyl)oxo(methoxycarbonylphenyl)methylaminodihydrofuran)

IT 101480-87-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with early bromide)

IT 101480-83-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)

RN 101480-83-5 HCAPLUS

CN Benzoic acid, 3-(1-cyano-2-oxo-3-phenylpropyl)-, methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 23 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:420516 HCAPLUS

DN 105:20516

ED Entered STN: 26 Jul 1986

TI 2-Substituted 5-amino-3-oxo-4-(substituted-phenyl)-2,3-dihydrofuran herbicides

IN Ward, Carl E.

PA Chevron Research Co. , USA

SO U.S., 13 pp.  
CODEN: USXXAM

DT Patent

LA English

IC ICM A01N043-08  
ICS C07D307-52

NCL 071088000

CC 5-3 (Agrochemical Bioregulators)  
Section cross-reference(s): 27

FAN.CNT 1

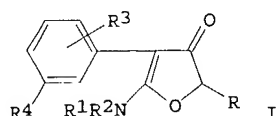
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4568375	A	19860204	US 1984-666075	19841026 <--
PRAI US 1984-666075		19841026 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4568375	ICM	A01N043-08
	ICS	C07D307-52
	NCL	071088000

OS CASREACT 105:20516

GI



AB The herbicidal title compds. I (R = halo, alkoxy, alkenylmethoxy; R1 = alkyl; R2 = alkyl, alkenyl, alkoxycarbonylalkyl, etc.; NR1R2 = ring; R3 = H, alkyl, halo, etc.; R4 = alkyl, haloalkyl, etc.) are prepared by halogenation of I (R = H) with a N-halosuccinimide, under UV light, followed eventually by alkylation. Thus, a solution of I (R = R3 = H, R1 = R2 = Me, R4 = 3-F3C(C6H4) (preparation given), N-bromosuccinimide and a small amount of Bz2O2 in C6H6 was irradiated with 300-600 nm light for 2 h, to give I (R = Br, R1 = R2 = Me, R3 = H, R4 = 3-F3(C6H4) which was reacted with EtONa, to give I (R = OEt, R1 = R2 = Me, R3 = H, R4 = F3C) (II). In pot expts., pre-emergence 27.5 .mu.g II/cm2 totally controlled crabgrass, wild oats, lambsquarters, mustard, and other weeds.

ST furanone herbicide prepn; halogenation furanone UV light

IT Halogenation

(of phenyldimethylaminodihydrofuranones, photochem.)

IT Herbicides  
(phenylaminodihydrofuranones)

IT 101480-91-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and bromination of)

IT 96541-98-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)

IT 101480-92-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and epoxylation of)

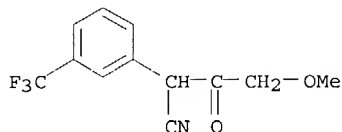
IT 96525-52-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and methylation)

IT 23145-00-8P 23145-02-0P 76996-63-9P 96541-91-2P 96541-92-3P  
96541-93-4P 96541-94-5P 96541-95-6P 96541-96-7P 96541-97-8P  
96572-49-5P 96572-50-8P 96572-51-9P 96906-18-2P 96906-20-6P  
96906-21-7P 101480-93-7P 101480-94-8P 101480-95-9P 101480-96-0P  
101480-97-1P 101480-98-2P 101504-44-3P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except  
adverse); BSU (Biological study, unclassified); SPN (Synthetic  
preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as herbicide)

IT 96541-98-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)

RN 96541-98-9 HCAPLUS

CN Benzeneacetonitrile, .alpha.-(methoxyacetyl)-3-(trifluoromethyl)- (9CI)  
(CA INDEX NAME)



L28 ANSWER 24 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:19417 HCAPLUS

DN 104:19417

ED Entered STN: 24 Jan 1986

TI Biocidal enol esters of non-ortho substituted 2-aryl-1,3-cycloalkanedione  
compounds

IN Wheeler, Thomas N.; Weiden, Mathias H. J.

PA Union Carbide Corp. , USA

SO U.S., 10 pp. Cont. of U.S. Ser. No. 946,311 abandoned.  
CODEN: USXXAM

DT Patent

LA English

IC ICM C11C003-04  
ICS C07C069-03

NCL 260410500

CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 5

FAN.CNT 1

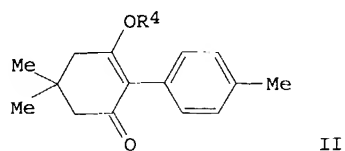
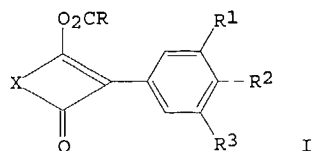
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4526723	A	19850702	US 1983-510731	19830705 <--
PRAI US 1978-946311		19780927 <--		

CLASS

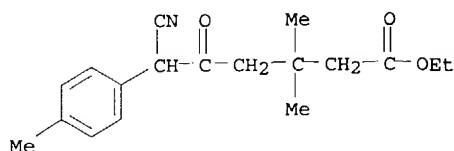
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4526723	ICM	C11C003-04
	ICS	C07C069-03
	NCL	260410500

OS CASREACT 104:19417

GI



- AB Title compds. I [R = (un)substituted alkyl, alkenyl, alkynyl, Ph, haloalkyl, cycloalkyl, cycloalkenyl, phenylalkyl; R1, R2, R3 = H, haloalkyl, halo, alkyl; X = (un)substituted C2, C3 alkylene], useful as acaricides and herbicides, were prepared. Thus, Et 3,3-dimethylglutarate reacted with 4-MeC6H4CH2CN to give 68% 4-MeC6H4CH(CN)COCH2CMe2CH2CO2Et, which cyclized to give 57% of the enol II (R4 = H). The last was treated with Me(CH2)6COCl to give II [R4 = CO(CH2)6Me] (III). At 2500 ppm preemergent, III gave complete inhibition of crabgrass (*Digitaria sanguinalis*) without damage to the tomatoes. III also gave excellent control of 2-spotted mites (*Tetranychus urticae*) as adults and eggs.
- ST acaricide arylcycloalkanedione enol ester prepn; herbicide arylcycloalkanedione enol ester prepn; arylcycloalkanedione enol ester acaricide herbicide; cycloalkanedione enol ester acaricide herbicide
- IT Acaricides  
Herbicides  
(aryl-cycloalkanedione enol esters)
- IT Enols  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(esters of, of arylcycloalkanediones, as acaricides and herbicides)
- IT Esters, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(of arylcycloalkanedione enols, preparation and acaricidal and herbicidal activity of)
- IT 99480-51-0P 99480-53-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of, to cyclohexanedione)
- IT 99480-52-1P 99480-54-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and esterification of, with alkanoyl chloride)
- IT 83786-58-7P 83786-59-8P 83786-60-1P 83786-61-2P 83786-62-3P  
83786-63-4P 83786-67-8P 99480-38-3P 99480-39-4P 99480-40-7P  
99480-41-8P 99480-42-9P 99480-43-0P 99480-44-1P 99480-45-2P  
99480-46-3P 99480-47-4P 99480-48-5P 99480-49-6P 99480-50-9P  
99480-55-4P 99480-56-5P 99480-57-6P 99480-58-7P 99480-59-8P  
99496-99-8P 99497-00-4P 99497-01-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, acaricidal, and herbicidal activity of)
- IT 17804-59-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with benzyl cyanide)
- IT 1529-41-5 2947-61-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with glutarate)
- IT 99480-51-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of, to cyclohexanedione)
- RN 99480-51-0 HCAPLUS
- CN Benzenehexanoic acid, .epsilon.-cyano-.beta.,.beta.,4-trimethyl-.delta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



ED Entered STN: 12 Jan 1985  
 TI Pesticidal cyano enol phosphates  
 IN D'Silva, Themistocles D. J.  
 PA Union Carbide Corp. , USA  
 SO U.S., 9 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A01N057-14; C07F009-165  
 NCL 424210000  
 CC 29-7 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 5

FAN.CNT 1

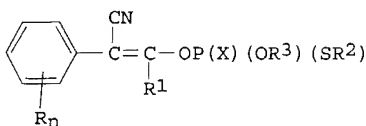
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4469688	A	19840904	US 1982-393552	19820630 <--
PRAI	US 1982-393552		19820630 <--		

CLASS

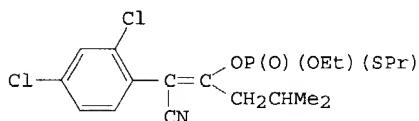
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4469688	IC NCL	A01N057-14IC 424210000

OS CASREACT 102:6812

GI



I



II

AB About 29 title compds. I [R = H, alkyl, alkylthio, alkoxy, trihalomethyl, di- or trifluoromethoxy, halo; R1 = H, (un)substituted alkyl, halocycloalkyl, alkenyl, alkenylcycloalkyl, alkynyl, trihaloalkyl, alkoxy carbonyl, PhCH2, alkyl, alkoxyalkyl, haloalkoxyalkyl, alkoxy carbonylalkyl, alkoxyphenyl, haloalkoxyphenyl, alkoxy carbonylphenyl; X = O; n = 0-5; R2 = Pr, R3 = Et], insecticides and miticides, were prepared Thus, treating 2,4-Cl2C6H3CH(CN)C(O)CH2CHMe2 in MeCN with ClP(O)(OEt)(SPr) gave 68% thiophosphate (II). Some examples of I were more effective against the two-spotted mite than Kelthane.

ST cyano enol phosphate insecticide; miticide cyano enol phosphate

IT Acaricides

Insecticides

(cyano enol phosphates)

IT	93502-43-3P	93502-44-4P	93502-45-5P	93502-46-6P	93502-47-7P
	93502-48-8P	93502-49-9P	93502-50-2P	93502-51-3P	93502-52-4P
	93502-53-5P	93502-54-6P	93502-55-7P	93502-56-8P	93502-57-9P
	93502-58-0P	93502-59-1P	93502-60-4P	93502-61-5P	93502-62-6P
	93502-63-7P	93502-64-8P	93502-65-9P	93502-66-0P	93502-67-1P
	93502-68-2P	93502-69-3P	93502-70-6P	93502-71-7P	

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and pesticidal activity of)

IT 93502-72-8P 93502-73-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with Et Pr chlorothiophosphate)

IT 71871-79-9 93502-74-0

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et Pr chlorothiophosphate)

IT 22364-68-7

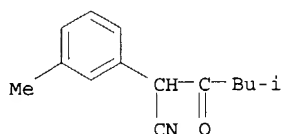
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et benzoate)

IT 2947-60-6

RL: RCT (Reactant); RACT (Reactant or reagent)



(reaction of, with Et isovalerate)  
 IT 7651-98-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with acyl-substituted benzyl cyanides)  
 IT 93-89-0 108-64-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with methylbenzyl cyanide)  
 IT 93502-72-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with Et Pr chlorothiophosphate)  
 RN 93502-72-8 HCAPLUS  
 CN Benzeneacetonitrile, 3-methyl-.alpha.-(3-methyl-1-oxobutyl)- (9CI) (CA  
 INDEX NAME)



L28 ANSWER 26 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1984:610574 HCAPLUS  
 DN 101:210574  
 TI Condensation of substituted phenylacetonitriles with dicarboxylic  
 anhydrides  
 IN Ligon, Robert C.  
 PA Union Carbide Corp. , USA  
 SO U.S., 3 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07C121-76  
 NCL 260465000D  
 CC 23-16 (Aliphatic Compounds)  
 Section cross-reference(s): 25

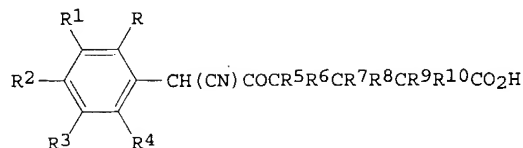
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4470929	A	19840911	US 1983-480733	19830331 <--
US 1983-480733		19830331 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4470929	IC	C07C121-76
	NCL	260465000D

GI



I

AB 6-Cyano-6-phenyl-5-oxohexanoic acids I [R = alkyl, halo, polyhaloalkyl, haloalkyl; R1, R2, R3, and R4 are H, NO2, polyhaloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino, haloalkyl; R5, R6, R7, R8, R9, and R10 are H, alkyl, Ph, alkyl-, cyano-, halo-, nitro-, alkoxy-, alkylthio-, alkylsulfinyl-, alkylsulfonyl-, or (dialkylamino)phenyl] were prepared from glutaric anhydrides, phenylacetonitriles, and bases. 3,3-Dimethylglutaric anhydride was heated with 2-MeC6H4CH2CN and NaNH2-NaOCMe3 in THF-Me3COH to give 2-MeC6H4CH(CN)COCH2CMe2CH2CO2H.  
 ST cyanophenyl-5-oxohexanoic acid; hexanoic acid cyano oxo phenyl; condensation glutaric anhydride catalyst; glutaric anhydride condensation phenylacetonitrile  
 IT Condensation reaction catalysts

(sodium alkoxides, for glutaric anhydride derivative with phenylacetonitrile derivative)

IT 865-48-5  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts from sodamide and, for condensation of glutaric anhydride derivative with phenylacetonitrile derivative)

IT 7782-92-5  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts from sodium tert-butoxide and, for condensation of glutaric anhydride derivative with phenylacetonitrile derivative)

IT 141-52-6  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for condensation of glutaric anhydride derivative with phenylacetonitrile derivative)

IT 22364-68-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with glutaric anhydride derivative, catalysts for)

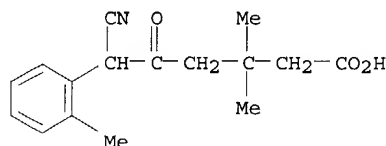
IT 4160-82-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with phenylacetonitrile derivative, catalysts for)

IT 93079-58-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 93079-58-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 93079-58-4 HCAPLUS

CN Benzenehexanoic acid, .epsilon.-cyano-.beta., .beta., 2-trimethyl-.delta.-oxo- (9CI) (CA INDEX NAME)



L28 ANSWER 27 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1984:610572 HCAPLUS

DN 101:210572

TI Condensation of ring-substituted phenylacetonitriles with monoesters of dicarboxylic acids

IN Ligon, Robert C.

PA Union Carbide Corp. , USA

SO U.S., 3 pp.  
CODEN: USXXAM

DT Patent

LA English

IC C07C121-76

NCL 260465000D

CC 23-16 (Aliphatic Compounds)  
Section cross-reference(s): 25

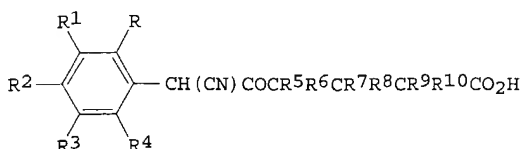
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4469642	A	19840904	US 1983-480726	19830331 <--
PRAI	US 1983-480726		19830331	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4469642	IC	C07C121-76
	NCL	260465000D

GI



I

AB The base-catalyzed reaction of phenylacetone nitriles with monoalkyl glutarates gave hexanoic acids I [R = alkyl, halo, polyhaloalkyl, haloalkyl; R1, R2, R3, and R4 are H, NH3, polyhaloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino, haloalkyl; R5, R6, R7, R8, R9, and R10 are H, alkyl, substituted alkyl, Ph, alkyl-, cyano-, halo-, nitro-, alkoxy-, (alkylthio)-, (alkylsulfinyl)-, (alkylsulfonyl)-, or (dialkylamino)phenyl]. Thus, 2-MeC6H4CH2CN underwent a condensation reaction with EtO2CCH2CMe3CH2CO2H and NaOEt to give I (R = R7 = R8 = Me, R1 = R2 = R3 = R4 = R5 = R6 = R9 = R10 = H).

ST butyric acid phenylcyanoacetyl; cyanophenylacetylbutyric acid; phenylcyanoacetylbutyric acid

IT Condensation reaction catalysts  
(sodium ethoxide, for phenylacetone nitrile derivative with monoethyl glutarate derivative)

IT 141-52-6  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for condensation of phenylacetone nitrile derivative with monoethyl glutarate derivative)

IT 22364-68-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with monoethyl glutarate derivative, catalysts for)

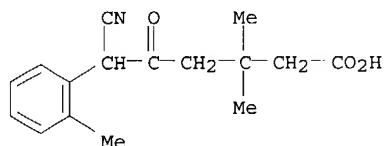
IT 93218-34-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with phenylacetone nitrile derivative, catalysts for)

IT 93079-58-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 93079-58-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 93079-58-4 HCAPLUS

CN Benzenhexanoic acid, .epsilon.-cyano-.beta.,.beta.,2-trimethyl-.delta.-oxo- (9CI) (CA INDEX NAME)



L28 ANSWER 28 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1982:544457 HCAPLUS

DN 97:144457

ED Entered STN: 12 May 1984

TI Biocidal 2-aryl-1,3-cyclopentanedione compounds and their alkali metal and ammonium salts

IN Wheeler, Thomas N.

PA Union Carbide Corp. , USA

SO U.S., 16 pp. Cont.-in-part of U.S. 4,283,348.  
CODEN: USXXAM

DT Patent

LA English

IC A61K031-12; C07C049-427; A01N031-00

NCL 071122000

CC 24-4 (Alicyclic Compounds)  
Section cross-reference(s): 5

FAN.CNT 2

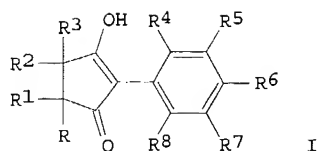
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4338122	A	19820706	US 1980-197600	19801016 <--
	US 4283348	A	19810811	US 1979-78923	19790926 <--
PRAI	US 1978-944995		19780922	<--	
	US 1979-78923		19790926	<--	

CLASS

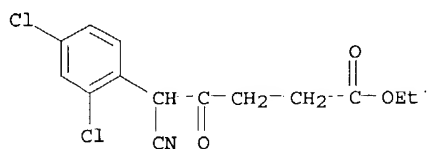
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4338122	IC	A61K031-12IC C07C049-427IC A01N031-00
	NCL	071122000

OS CASREACT 97:144457

GI



- AB Title compds. I [R, R1, R2, and R3 individually are H, (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, or Ph, or any two of R, R1, R2, and R3 form an alkylene or alkenylene bridge; R4 = alkyl, haloalkyl, halo; R5, R6, R7, and R8 individually are H, NO2, haloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino] were prepared, and they exhibited herbicidal and acaricidal activity. Thus, 2,4-Cl2C6H3CH2CN was acylated by EtO2CCH2CH2CO2Et, the product was converted to 2,4-Cl2C6H3CH2COCH2CH2CO2Et, and the latter was heated with Na in EtOH to give 2-(2,4-dichlorophenyl)-1,3-cyclopentanedione.
- ST phenylcyclopentanedione prepn herbicide acaricide; cyclopentanedione phenyl prepn herbicide
- IT Acaricides  
Herbicides  
(phenylcyclopentanediones and perhydroindandione analogs)
- IT 4676-51-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation by, of phenylacetone nitrile derivative)
- IT 123-25-1 10138-59-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation by, of phenylacetone nitriles)
- IT 6306-60-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of, by succinate ester)
- IT 22364-68-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of, by succinate ester derivative)
- IT 16213-85-7 68429-53-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of, by succinate esters)
- IT 83190-41-4  
RL: PROC (Process)  
(addition of, with benzaldehyde derivative)
- IT 874-42-0  
RL: PROC (Process)  
(addition of, with bicyclooctenone derivative)
- IT 80036-04-0P 83190-40-3P 83190-42-5P 83190-43-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and conversion of, to indandione derivative)
- IT 80035-92-3P 80035-98-9P 80035-99-0P 80036-08-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation of)
- IT 80035-91-2P 80035-96-7P 80035-97-8P 80036-07-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and esterification of, by ethanol)
- IT 80035-93-4P 80036-00-6P 80036-03-9P 80036-05-1P 80036-09-5P  
80036-11-9P 80036-14-2P 80036-15-3P 80036-16-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and herbicidal and acaricidal activity of)
- IT 80035-90-1P 80035-94-5P 80035-95-6P  
80036-01-7P 80036-06-2P 80036-10-8P  
80036-13-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis-decarboxylation of)
- IT 80035-90-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis-decarboxylation of)
- RN 80035-90-1 HCAPLUS
- CN Benzenepentanoic acid, 2,4-dichloro-.delta.-cyano-.gamma.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 29 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1982:6260 HCAPLUS

DN 96:6260

ED Entered STN: 12 May 1984

TI 2-Aryl-1,3-cyclopentanedione compounds

IN Wheeler, Thomas N.

PA Union Carbide Corp. , USA

SO U.S., 12 pp. Division of U.S. Ser. No. 944,995.

CODEN: USXXAM

DT Patent

LA English

IC C07C049-707; C07C121-76; C07C147-10

NCL 260465000D

CC 24-4 (Alicyclic Compounds)

Section cross-reference(s): 5, 25

FAN.CNT 2

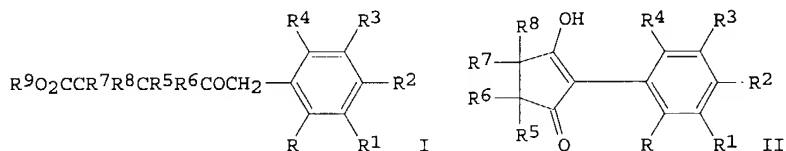
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4283348	A	19810811	US 1979-78923	19790926 <--
	US 4338122	A	19820706	US 1980-197600	19801016 <--
PRAI	US 1978-944995		19780922	<--	
	US 1979-78923		19790926	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4283348	IC	C07C049-707IC C07C121-76IC C07C147-10
	NCL	260465000D

OS CASREACT 96:6260

GI



AB 4-Oxopentanoate esters I [R = alkyl, haloalkyl, halo, polyhaloalkyl; R1, R2, R3, and R4 individually are H, NO2, polyhaloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino, haloalkyl; R5, R6, R7, and R8 individually are H, (un)substituted alkyl, alkenyl, cycloalkyl, or cycloalkenyl, Ph, alkyl-, alkanoyl-, cycloalkyl-, cycloalkenyl-, cyano-, halo-, nitro-, alkoxy-, aryloxy-, alkylthio-, arylthio-, alkylsulfinyl-, alkylsulfonyl-, (acylamino)-, or (dialkylamino)phenyl; R9 = alkyl] were treated with NaOEt at 100-25.degree. to yield title compds. II, which exhibited acaricidal and herbicidal activity. Thus, 2,4-Cl2C6H3CH2CN was acylated by EtO2CCH2CH2CO2Et and the product was converted to EtO2CCH2CH2COCH2C6H3Cl2-2,4 (III) in two steps, and III (in PhMe) was heated with Na in EtOH at .apprx.100.degree. to give 2-(2,4-dichlorophenyl)-1,3-cyclopentanedione.

ST phenylcyclopentanedione prepn acaricide herbicide; cyclopentanedione phenyl prepn herbicide

IT Acaricides

Herbicides

(phenylcyclopentanediones and phenylhexahydroindanones)

IT 123-25-1 10138-59-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(acylation of phenylacetonitriles by)

IT 22364-68-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(acylation of, by diethylsuccinate derivative)

IT 4676-51-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of, by phenylacetone nitrile derivative)

IT 6306-60-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of, by succinate ester)

IT 16213-85-7 68429-53-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of, by succinate ester derivs.)

IT 36461-33-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(addition reaction of, with benzaldehyde derivative)

IT 874-42-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(addition reaction of, with cyclobutenediol disilyl ether derivative)

IT 80035-93-4P 80036-00-6P 80036-03-9P 80036-05-1P 80036-09-5P  
80036-11-9P 80036-14-2P 80036-15-3P 80036-16-4P 80036-17-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and acaricidal and herbicidal activity of)

IT 80035-92-3P 80035-98-9P 80035-99-0P 80036-06-2P  
80036-08-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation reaction of)

IT 80035-91-2P 80035-96-7P 80035-97-8P 80036-07-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and esterification of, by ethanol)

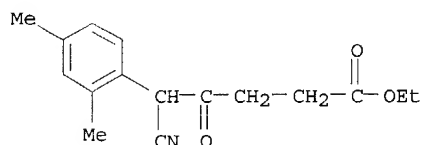
IT 80035-90-1P 80035-94-5P 80035-95-6P  
80036-01-7P 80036-10-8P 80036-13-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of, decarboxylation in)

IT 80036-02-8P 80036-04-0P 80036-12-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and rearrangement of indandione analog from)

IT 80036-06-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation reaction of)

RN 80036-06-2 HCAPLUS

CN Benzenepentanoic acid, .delta.-cyano-2,4-dimethyl-.gamma.-oxo-, ethyl  
ester (9CI) (CA INDEX NAME)



L28 ANSWER 30 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1981:603926 HCAPLUS  
DN 95:203926  
ED Entered STN: 12 May 1984  
TI Substituted isoxazolines for control of plant phytopathogens  
IN Davenport, James D.  
PA Eli Lilly and Co., USA  
SO U.S., 5,668, abandoned.  
CODEN: USXXAM  
DT Patent  
LA English  
IC C07D413-04; A01N043-80  
NCL 424263000  
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 5  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4283403	A	19810811	US 1977-829304	19770831 <--
	IL 51948	A1	19800630	IL 1977-51948	19770426 <--
	CA 1082185	A1	19800722	CA 1977-277139	19770427 <--
	GB 1581583	A	19801217	GB 1977-24189	19770609 <--

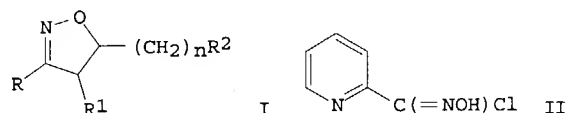
BE 855602	A1	19771212	BE 1977-8185	19770610 <--
JP 52153959	A2	19771221	JP 1977-70432	19770613 <--
FR 2355010	A1	19780113	FR 1977-18050	19770613 <--
FR 2355010	B1	19800201		
BR 7703803	A	19780418	BR 1977-3803	19770613 <--
NL 7706558	A	19771216	NL 1977-6558	19770614 <--
BR 7703863	A	19780425	BR 1977-3863	19770614 <--
CH 627049	A	19811231	CH 1977-7307	19770614 <--
PRAI US 1976-695668		19760614	<--	

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4283403	IC	C07D413-04IC A01N043-80
	NCL	424263000

OS CASREACT 95:203926

GI



- AB 2-Isloxazolines I (R = 2-pyridyl; R1 = H, Ph; n = 1, 2; R2 = isothiocyanato) were prepared and exhibited fungicidal activity. Thus, treating imidoyl chloride II, prepared from the aldoxime, with CH2:CHCH2NCS and Et3N gave I (R = 2-pyridyl, R1 = H, n = 1, R2 = isothiocyanato). Similarly prepared were I (R = Ph, alkoxy-, nitro-, alkyl-, or halophenyl; R1 = H, Ph; n = 1, 2; R2 = isothiocyanato, cyano, NH2) which also showed fungicidal activity.
- ST isoxazoline isothiocyanatomethyl prepn fungicide;  
isothiocyanatomethylisoxazoline prepn fungicide
- IT Fungicides and Fungistats  
((isothiocyanatoalkyl)isoxazolines)
- IT 110-91-8, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(addition reaction of, with (isothiocyanatoalkyl)isoxazolines)
- IT 74-89-5, reactions 108-18-9 302-01-2, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(addition reaction of, with (isothiocyanatomethyl)isoxazoline derivs.)
- IT 932-90-1  
RL: PROC (Process)  
(conversion of, to N-hydroxybenzamidoyl chloride)
- IT 459-23-4 3235-02-7 25185-95-9 34158-73-1 56843-28-8  
RL: PROC (Process)  
(conversion of, to N-hydroxybenzimidoyl chloride derivative)
- IT 3235-04-9  
RL: PROC (Process)  
(conversion of, to N-hydroxybenzimidoyl chlorides)
- IT 873-69-8  
RL: PROC (Process)  
(conversion of, to N-hydroxyimidoyl chloride analog)
- IT 3717-28-0 29203-59-6 65788-66-1 65788-68-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. reaction of, with allyl isothiocyanate)
- IT 109-75-1 19364-21-7 65788-85-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. reaction of, with N-hydroxybenzimidoyl chloride)
- IT 2253-93-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. reaction of, with N-hydroxybenzimidoyl chlorides)
- IT 57-06-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. reaction of, with N-hydroxybenzimidoyl chlorides, isoxazolines from)
- IT 104-88-1, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oximation of)
- IT 122-03-2 454-89-7 455-19-6 555-16-8, reactions 3218-36-8 6502-22-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oximation of, and conversion of product to N-hydroxybenzimidoyl chloride derivative)

IT 4397-53-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oximation of, and conversion of products to N-hydroxybenzimidoyl  
 chlorides)

IT 3848-36-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and conversion of, to N-hydroxybenzimidoyl chloride derivative)

IT 698-16-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and cycloaddn. reaction of, with alkenyl isothiocyanates, allyl  
 cyanide and allylamine derivs.)

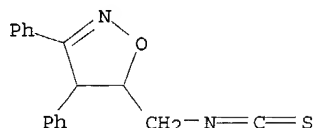
IT 42202-94-8P 42202-95-9P 61946-90-5P 65788-87-6P 65788-96-7P  
 69716-28-5P 79754-91-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and cycloaddn. reaction of, with allyl isothiocyanate)

IT 1011-84-3P 6579-27-7P 28123-63-9P 29203-60-9P 33126-97-5P  
 36288-37-6P 38435-51-7P 69053-93-6P 74467-05-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and cycloaddn. reaction of, with aryl isothiocyanate)

IT 6501-74-2P 14654-87-6P 65788-61-6P 65788-62-7P 65788-63-8P  
 65788-64-9P 65788-67-2P 65788-69-4P 65788-70-7P 65788-71-8P  
 65788-72-9P 65788-73-0P 65788-74-1P 65788-75-2P 65788-76-3P  
 65788-77-4P 65788-78-5P 65788-79-6P 65788-80-9P 65788-81-0P  
 65788-82-1P 65788-83-2P 65788-86-5P 65788-88-7P  
 65788-92-3P 65788-93-4P 65788-94-5P 65788-95-6P 65991-25-5P  
 79754-92-0P 79754-93-1P 79754-94-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (preparation and fungicidal activity of)

IT 65788-86-5P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (preparation and fungicidal activity of)

RN 65788-86-5 HCAPLUS  
 CN Isoxazole, 4,5-dihydro-5-(isothiocyanatomethyl)-3,4-diphenyl- (9CI) (CA  
 INDEX NAME)



L28 ANSWER 31 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1981:84125 HCAPLUS  
 DN 94:84125  
 ED Entered STN: 12 May 1984  
 TI Substituted arylcyanoalkyl and diaryl cyanoalkylimidazoles  
 IN Miller, George A.; Chan, Hak-Foon; Carley, Harold E.  
 PA Rohm and Haas Co., USA  
 SO U.S., 18 pp. Cont.-in-part of U.S. 4,143,137.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07D233-90  
 NCL 548341000  
 CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 5  
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4225723	A	19800930	US 1979-1658	19790108 <--
	US 4073921	A	19780214	US 1976-647039	19760107 <--
	CA 1067903	A1	19791211	CA 1976-244896	19760203 <--
	CH 621777	A	19810227	CH 1976-1354	19760204 <--
	AT 7600810	A	19791115	AT 1976-810	19760205 <--
	AT 357365	B	19800710		
	PL 107215	P	19800229	PL 1976-187683	19760303 <--

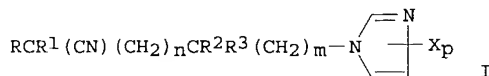


PL 123447	B1	19821030	PL 1976-200363	19760303 <--
US 4143137	A	19790306	US 1977-839877	19771006 <--
FR 2384761	A1	19781020	FR 1978-4787	19780220 <--
FR 2384761	B1	19800829		
PRAI US 1975-557546		19750312 <--		
US 1976-647039		19760107 <--		
US 1977-839877		19771006 <--		

## CLASS

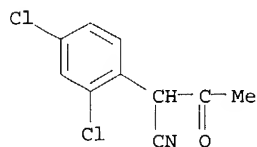
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4225723	IC	C07D233-90
	NCL	548341000

GI



- AB 1-Unsubstituted imidazoles were N-alkylated by arylcyanoalkyl halides and mesylates and NaH, NaOH, or quaternary ammonium halides to yield 1-(arylcyanoalkyl)imidazoles I [R = aryl, halo-, nitro-, cyano-, alkoxy-, alkyl-, (trihalomethyl)-, benzyl-, or phenylaryl, or CRR1 = fluorenylidene; R1 = alkyl, cycloalkyl, alkenyl, cycloalkenyl, alkynyl, Ph, halo-, nitro-, cyano-, alkoxy-, alkyl-, or (trihalomethyl)phenyl, (un)substituted benzyl, (un)substituted phenethyl; n = 0, 1, 2, 3, 4, 5; R2 and R3 are independently H, alkyl, Ph, halo-, nitro-, cyano-, alkoxy-, alkyl-, or (trihalomethyl)phenyl, (un)substituted benzyl, (un)substituted phenethyl; m = 0, 1, 2, 3, 4, 5; p = 0, 1, 2 (X = halo)], which showed fungicidal activity. Thus, 2,4-Cl2C6H3CHBuCN was hydroxymethylated by paraformaldehyde, the product was converted to 2-cyano-2-(2,4-dichlorophenyl)hexyl mesylate (II), and imidazole reacted with II to give I (n = m = p = 0, R = 2,4-Cl2C6H3, R1 = Bu, R2 = R3 = H).
- ST arylcyanoalkylimidazole prepn fungicide; imidazole arylcyanoalkyl prepn fungicide
- IT Fungicides and Fungistats  
(N-(phenylcyanoalkyl)imidazoles)
- IT 89-98-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction of, with bromochlorobenzene)
- IT 106-39-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction of, with chlorobenzaldehyde)
- IT 61019-78-1P 61019-79-2P 61019-81-6P 61019-82-7P 61019-83-8P  
61019-85-0P 61019-86-1P 61019-87-2P 61019-88-3P 61019-89-4P  
61019-90-7P 61019-91-8P 61019-92-9P 61019-93-0P 61019-94-1P  
61019-96-3P 61023-03-8P 61023-04-9P 61023-05-0P 61023-06-1P  
61023-09-4P 61023-10-7P 61023-11-8P 61023-12-9P 61023-13-0P  
61023-15-2P 61023-17-4P 61023-18-5P 61023-19-6P 61023-20-9P  
61023-21-0P 61023-22-1P 61023-24-3P 61023-26-5P 61023-28-7P  
61023-30-1P 61023-31-2P 61023-33-4P 61023-34-5P 61023-35-6P  
61023-36-7P 61023-37-8P 61023-38-9P 61023-39-0P 61023-40-3P  
61023-41-4P 61023-42-5P 61023-43-6P 61023-44-7P 61023-45-8P  
61023-46-9P 61023-92-5P 61055-47-8P 61055-49-0P 61055-50-3P  
76562-08-8P 76562-10-2P 76562-11-3P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation and fungicidal activity of)
- IT 43171-49-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with phosphorus tribromide)
- IT 61023-86-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and substitution reaction of, with cuprous cyanide)
- IT 3508-98-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and .alpha.-chloromethylation of)
- IT 58830-59-4P 58830-64-1P 59666-80-7P 61023-87-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)  
 (preparation and .alpha.-hydroxymethylation of)  
 IT 61023-79-8P 61023-82-3P 61023-84-5P 61023-88-9P 61023-90-3P  
 61023-93-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and O-mesylation of)  
 IT 76562-14-6P 76562-15-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 61023-80-1P 61023-81-2P 61023-83-4P 61023-85-6P 61023-89-0P  
 61023-91-4P 61023-94-7P 76562-12-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, and N-alkylation of imidazole by)  
 IT 20968-04-1P 58830-65-2P 63866-57-9P 76562-13-5P 76562-16-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, for N-alkylation of imidazole)  
 IT 140-29-4 6306-60-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-alkylation of)  
 IT 109-69-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-alkylation of phenylacetonitrile by)  
 IT 103-63-9 111-24-0 111-83-1 542-69-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-alkylation of phenylacetonitrile derivative by)  
 IT 75-09-2, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-chloromethylation of phenylacetonitrile derivative by)  
 IT 2184-88-5 5005-36-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-hydroxymethylation of)  
 IT 30525-89-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-hydroxymethylation of phenylacetonitriles by)  
 IT 288-32-4, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (N-alkylation of, by phenylalkyl mesylates)  
 IT 76562-15-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 76562-15-7 HCAPLUS  
 CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dichloro- (9CI) (CA INDEX NAME)



L28 ANSWER 32 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1981:30760 HCAPLUS  
 DN 94:30760  
 ED Entered STN: 12 May 1984  
 TI Substituted 6-phenyl-1,2,4-triazolo[4,3-a]pyridines  
 IN Albright, Jay D.; Trust, Ronald I.  
 PA American Cyanamid Co., USA  
 SO U.S., 11 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07D471-04; A61K031-44  
 NCL 546119000  
 CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 27

FAN.CNT 1

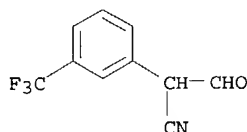
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4209626	A	19800624	US 1979-20886	19790315 <--
PRAI US 1979-20886		19790315 <--		

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

Searched by Noble Jarrell

(Reactant or reagent)  
 (preparation and decarboxylation of)  
 IT 76053-48-0P 76053-49-1P 76053-50-4P 76066-36-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and hydrazinolysis of)  
 IT 76066-49-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and hydrogenation of)  
 IT 35982-93-5P 35982-98-0P 59198-14-0P 76053-34-4P 76053-35-5P  
 76053-36-6P 76053-37-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and hydrolysis of)  
 IT 15131-89-2P 19927-64-1P 59198-06-0P 76053-33-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction of, with cyanoacetamide)  
 IT 76053-41-3 76053-42-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation decarboxylation of)  
 IT 2338-76-3P 10177-08-9P 70806-40-5P 76053-40-2P 76053-45-7P  
 76053-47-9P 76066-42-7P 76066-43-8P 76066-44-9P 76066-45-0P  
 76066-46-1P 76066-48-3P 76066-51-8P 76066-52-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 64-19-7, reactions 331-25-9 351-35-9 1878-66-6 2444-36-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with DMF)  
 IT 109-94-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with benzeneacetonitrile derivative)  
 IT 68-12-2, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetates)  
 IT 70806-40-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 70806-40-5 HCAPLUS  
 CN Benzeneacetonitrile, .alpha.-formyl-3-(trifluoromethyl)- (9CI) (CA INDEX  
 NAME)



L28 ANSWER 33 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1980:568298 HCAPLUS

DN 93:168298

ED Entered STN: 12 May 1984

TI (Substituted-phenyl)-1,2,4-triazolo[4,3-a]pyrimidines and  
 (substituted-phenyl)-1,2,4-triazolo[1,5-a]pyrimidines

IN Albright, Jay D.; Dusza, John P.; Hardy, Robert A., Jr.

PA American Cyanamid Co., USA

SO U.S., 12 pp.

CODEN: USXXAM

DT Patent

LA English

IC A61K031-505; C07D487-04

NCL 544263000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

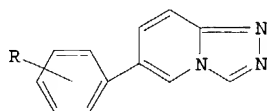
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4209621	A	19800624	US 1979-34060	19790427 <--
PRAI US 1979-34060		19790427 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES

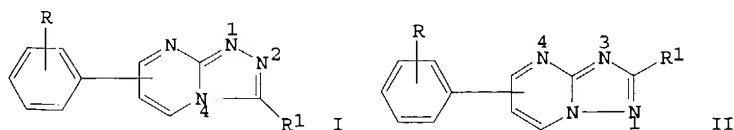
US 4209626 IC C07D471-04IC A61K031-44  
 NCL 546119000  
 GI



I

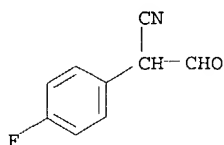
- AB Triazolopyridines I (R = H, C1-4 alkyl, C1-4 alkoxy, F, Cl, Br, CF<sub>3</sub>, cyano, CO<sub>2</sub>H, C2-5 alkoxy, carbonyl, CONH<sub>2</sub>, NO<sub>2</sub>, NH<sub>2</sub>, AcNH, C1-4 alkylamino, dialkylamino), useful as antihypertensives (no data), were prepared Thus, 4-ClC<sub>6</sub>H<sub>4</sub>C(CHO):CHNMe<sub>2</sub>, prepared by the condensation of DMF and 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H in the presence of POCl<sub>3</sub>, was cyclocondensed with NCCH<sub>2</sub>CONH<sub>2</sub>, hydrolyzed, decarboxylated, chlorinated by POCl<sub>3</sub>, and hydrazinolized to give 5-(4-chlorophenyl)-2-hydrazinopyridine (II). The cyclocondensation of II and HC(OEt)<sub>3</sub> gave I (R = 4-Cl).
- ST propenal phenylamino prepn cyclocondensation cyanoacetamide; hydrazinophenylpyridine prepn cyclocondensation orthoformate; pyridine hydrazinophenyl prepn cyclocondensation orthoformate; malonamide phenylpropenal cyclocondensation; formylhydrazine chlorophenylpyridine cyclocondensation; triazolopyridine prepn antihypertensive
- IT Antihypertensives  
 (phenyl-1,2,4-triazolo[4,3-a]pyridines)
- IT 108-59-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with aminophenylpropenal)
- IT 108-59-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with aminophenylpropenal)
- IT 624-84-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with chloro(chlorophenyl)pyridine)
- IT 53868-37-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with cyanoacetamide)
- IT 22252-94-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with di-Me malonate)
- IT 76066-36-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with formylhydrazine)
- IT 107-91-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with phenyl(dimethylamino)propenals)
- IT 122-51-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with phenylhydrazinopyridines)
- IT 105-53-3 108-13-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with phenylpropenal derivative)
- IT 66600-05-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrazinolysis of)
- IT 76066-47-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis of)
- IT 76053-43-5P 76053-44-6P 76053-46-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and chlorination of)
- IT 76066-37-0P 76066-38-1P 76066-39-2P 76066-40-5P 76066-41-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation of, with Et orthoformate)
- IT 76066-50-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation of, with di-Me malonate)
- IT 10177-08-9P 76053-38-8P 76053-39-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

US 4209621 IC A61K031-505IC C07D487-04  
 NCL 544263000  
 GI



- AB 2-Hydrazinopyrimidines underwent a cyclocondensation reaction with ortho esters to give triazolo[4,3-a]pyrimidines I (R = Cl, F, CF<sub>3</sub>, alkoxy; R<sub>1</sub> = H, alkyl), and triazolo[1,5-a]pyrimidines II (R and R<sub>1</sub> same as above) were prepared by the reaction of .beta.-aminoacrylophenones with 3-amino-1,2,4-triazole; I and II are useful as anxiolytic agents (no data). A mixture of 2-hydrazino-5-phenylpyrimidine and HC(OEt)<sub>3</sub> was refluxed 16 h to give 6-phenyl-[1,2,4]triazolo[4,3-a]pyrimidine.
- ST phenyltriazolopyrimidine prepn anxiolytic; triazolopyrimidine phenyl prepn anxiolytic
- IT Anxiety  
 (phenyltriazolopyrimidines effect on)
- IT 99-02-5 99-91-2 100-06-1 349-76-8 403-42-9 445-27-2 586-37-8  
 2142-68-9 17408-14-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation reaction of, with DMF di-Me acetal)
- IT 4637-24-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation reaction of, with acetophenones)
- IT 1201-93-0 1717-42-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reaction of, with aminotriazole)
- IT 35260-96-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reaction of, with hydrazine)
- IT 78-39-7 115-80-0 122-51-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reaction of, with hydrazinopyrimidines)
- IT 57-13-6, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reaction of, with .alpha.-(iminomethyl)phenylacetaldehydes, pyrimidines from)
- IT 4923-01-7 22819-05-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reaction of, with .beta.-aminoacrylophenone derivative)
- IT 62-56-6, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reaction of, with .beta.-aminoacrylophenones)
- IT 61-82-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation reactions of, with (aminomethylene)phenylacetaldehydes and .beta.-aminoacrylophenones)
- IT 62041-46-7P 72851-51-5P 75175-76-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation reaction of, with aminotriazole)
- IT 72851-19-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation reaction of, with aminotriazoles)
- IT 71734-79-7P 75175-43-8P 75175-44-9P 75175-46-1P 75175-47-2P  
 75175-48-3P 75175-49-4P 75175-50-7P 75175-90-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation reaction of, with ortho esters)
- IT 75175-45-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclocondensation reaction of, with orthoacetate ester)
- IT 51777-47-0P 75175-26-7P 75175-27-8P 75175-28-9P 75175-29-0P  
 75175-30-3P 75175-31-4P 75175-32-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation reaction of, with urea)  
 IT 27956-39-4P 56863-46-8P 74963-17-0P 75175-33-6P 75175-35-8P  
 75175-36-9P 75175-37-0P 75175-38-1P 75175-84-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction of, with phosphoryl chloride)  
 IT 75175-85-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reductive dechlorination of)  
 IT 398-42-5P 5841-70-3P 62538-21-0P  
 66154-58-3P 70806-40-5P 75175-23-4P  
 75175-24-5P 75175-25-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and selective hydrogenation of)  
 IT 22536-62-5P 27956-40-7P 56734-11-3P 74963-13-6P 75175-39-2P  
 75175-40-5P 75175-41-6P 75175-42-7P 75175-89-2P 75185-49-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and substitution reaction of, with hydrazine)  
 IT 2338-75-2P 2338-76-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and .alpha.-formylation of)  
 IT 60414-59-7P 75175-87-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and S-methylation of)  
 IT 56734-10-2P 75175-88-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and S-oxidation of)  
 IT 3038-47-9P 18096-70-3P 28587-05-5P 39573-72-3P 63680-91-1P  
 72851-21-9P 72851-22-0P 75175-34-7P 75175-51-8P 75175-52-9P  
 75175-53-0P 75175-54-1P 75175-55-2P 75175-56-3P 75175-57-4P  
 75175-58-5P 75175-59-6P 75175-60-9P 75175-61-0P 75175-62-1P  
 75175-63-2P 75175-64-3P 75175-65-4P 75175-66-5P 75175-67-6P  
 75175-68-7P 75175-69-8P 75175-70-1P 75175-71-2P 75175-72-3P  
 75175-73-4P 75175-74-5P 75175-75-6P 75175-77-8P 75175-78-9P  
 75175-79-0P 75175-80-3P 75175-81-4P 75175-82-5P 75175-83-6P  
 75175-86-9P 75175-91-6P 75175-92-7P 75175-93-8P 75175-94-9P  
 75175-95-0P 75175-96-1P 75185-50-1P 75185-51-2P 75185-52-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 302-01-2, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution reaction of, with chloropyrimidines)  
 IT 395-44-8 402-23-3 402-49-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution reaction of, with potassium cyanide)  
 IT 109-94-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-acylation of phenylacetonitriles by)  
 IT 140-29-4 140-53-4 459-22-3 501-00-8 1529-41-5 2856-63-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-formylation of)  
 IT 74-88-4, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (S-alkylation of pyrimidinethiols by)  
 IT 398-42-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and selective hydrogenation of)  
 RN 398-42-5 HCAPLUS  
 CN Benzeneacetonitrile, 4-fluoro-.alpha.-formyl- (9CI) (CA INDEX NAME)



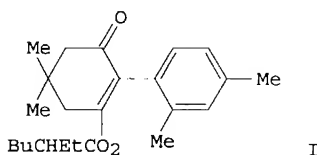
L28 ANSWER 34 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1980:400924 HCAPLUS  
 DN 93:924  
 ED Entered STN: 12 May 1984  
 TI Controlling acarina ectoparasites on warmblooded animals by orally  
 administering to the animal an ectoparasitically-effective amount of a  
 2-aryl-1,3-cyclohexanedione compound, and alkali metal salts, ammonium  
 salts and enol esters  
 IN Haines, Robert G.  
 PA Union Carbide Corp., USA  
 SO U.S., 17 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A61K031-22; A61K031-12; A61K031-275  
 NCL 424311000  
 CC 1-5 (Pharmacodynamics)  
 Section cross-reference(s): 25  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4175135	A	19791120	US 1978-925814	19780718 <--
	ZA 7903507	A	19800730	ZA 1979-3507	19790712 <--
	AU 7948939	A1	19800124	AU 1979-48939	19790716 <--
	AU 529257	B2	19830602		
	DK 7902990	A	19800119	DK 1979-2990	19790717 <--
	EP 7243	A1	19800123	EP 1979-301409	19790717 <--
	EP 7243	B1	19821117		
	R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AT 1813	E	19821215	AT 1979-301409	19790717 <--
	FI 7902259	A	19800119	FI 1979-2259	19790718 <--
	CA 1150626	A1	19830726	CA 1979-332184	19790719 <--
PRAI	US 1978-925814		19780718	<--	
	EP 1979-301409		19790717	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4175135	IC	A61K031-22IC A61K031-12IC A61K031-275
	NCL	424311000

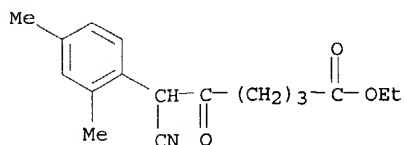
GI



AB 2-Aryl-1,3-cyclohexanediones are effective against ticks when given orally. Thus, 3-(2-ethylhexanoyloxy)-5,5-dimethyl-2(2',4'-dimethylphenyl)-2-cyclohexenone (I) [68427-67-8] was effective against *Dermacentor variabilis*, *Amblyomma americanum*, and *Amblyomma maculatum* when given orally to sheep at 7.0 mg/kg/day.

ST arylcyclohexanedione tick  
 IT Acaricides  
 (aryl-cyclohexanediones as)  
 IT 68427-46-3 72619-67-1 72619-68-2  
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)  
 (acaricidal activity of)  
 IT 68429-54-9 72619-69-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of)  
 IT 493-72-1 68429-52-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (diazotization of)  
 IT 30581-70-5DP, aryl derivs. 68427-67-8P  
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

- (preparation and acaricidal activity of)
- IT 68427-39-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and chlorination of)
- IT 68427-43-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and deamination of)
- IT 68429-55-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)
- IT 68427-48-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with mesitylene)
- IT 68427-51-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with toluene)
- IT 68427-38-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)
- IT 68427-39-4P 68427-40-7P 68427-41-8P 68427-42-9P 68427-44-1P  
68427-46-3P 68427-47-4P 68427-49-6P 68427-50-9P 68427-52-1P  
68427-53-2P 68427-55-4P 68427-56-5P 68427-57-6P  
68427-59-8P 68427-60-1P 68427-61-2P 68427-62-3P  
68427-64-5P 68427-65-6P 68427-66-7P 68427-68-9P 68427-69-0P  
71885-47-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 760-67-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with chlorophenyldimethylcyclohexanedione)
- IT 108-67-8, biological studies  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diazocyclohexanedione)
- IT 126-81-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with dichloronitrobenzene)
- IT 1460-08-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with mesitylene)
- IT 1807-68-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with xylene)
- IT 68429-55-0P  
RL: SPN (Synthetic preparation); PREP (Preparation);  
PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)
- RN 68429-55-0 HCAPLUS
- CN Benzenehexanoic acid, .epsilon.-cyano-2,4-dimethyl-.delta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 35 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1978:546892 HCAPLUS  
DN 89:146892  
ED Entered STN: 12 May 1984  
TI Isoxazolines  
IN Duranleau, Roger G.  
PA Texaco Inc., USA  
SO U.S., 4 pp.  
CODEN: USXXAM  
DT Patent

Searched by Noble Jarrell



LA English  
 IC C07D261-20  
 NCL 260307000DA  
 CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 40

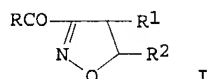
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4092327	A	19780530	US 1976-738996	19761105 <--
PRAI US 1976-738996		19761105 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4092327	IC	C07D261-20
	NCL	260307000DA

GI



AB Isoxazolines I (R = C1-20 alkyl, aryl; R1, R2 = H, C1-18 alkyl, C2-18 alkylene, aryl or R1R2 = polymethylene) were prepared by cyclocondensation of R1CH:CHR2 with RCOCH2NO2. Thus, Me(CH2)5CH:CH2 and Me(CH2)11COCH2NO2 heated at reflux in PhMe containing p-MeC6H4SO3H 7.5 h gave I [R = Me(CH2)11, R1 = H, R2 = hexyl]. I were useful as intermediates for photog. sensitizers.

ST isoxazoline acyl alkyl; alkanone isoxazolinyl

IT Alkenes, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with .alpha.-nitro ketones)

IT Cyclocondensation reaction

(of alkenes with .alpha.-nitro ketones)

IT Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (.alpha.-nitro, cyclocondensation of, with alkenes)

IT 10230-68-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with 1,2-diphenylethylene)

IT 55601-76-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with 1-octene)

IT 54044-25-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with 2-pentene)

IT 13291-54-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with cyclohexene)

IT 100-42-5, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with nitroacetophenone)

IT 109-68-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with nitrodecanone)

IT 110-83-8, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with nitrohexadecanone)

IT 588-59-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with nitropropanone)

IT 111-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with nitrotetradecanone)

IT 614-21-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with styrene)

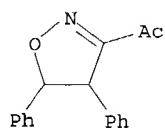
IT 7064-02-0P 67743-77-5P 67743-78-6P 67743-79-7P 67743-80-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 67743-78-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 67743-78-6 HCAPLUS  
 CN Ethanone, 1-(4,5-dihydro-4,5-diphenyl-3-isoxazolyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 36 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1977:584219 HCAPLUS

DN 87:184219  
 ED Entered STN: 12 May 1984  
 TI 1,4-Bis(arylacetyl)benzenes  
 IN Harris, Frank W.; Reinhardt, Bruce A.  
 PA Wright State University, USA  
 SO U.S., 5 pp.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC C07C049-76  
 NCL 260590000E  
 CC 25-16 (Noncondensed Aromatic Compounds)  
 Section cross-reference(s): 27

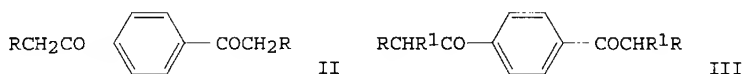
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4046814	A	19770906	US 1975-641959	19751218 <--
PRAI US 1975-641959		19751218 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4046814	IC	C07C049-76
	NCL	260590000E

GI



AB Terephthalic acid (I) derivs. were converted to diketones II (R = Ph, 2-pyridyl). I di-Me ester condensed with PhCH2CN and the III (R = Ph, R1 = CN) product was hydrolyzed and decarboxylated to give II (R = Ph). III (R = 2-pyridyl, R1 = CO2Et), which was prepared from I acid chloride and Et (2-pyridyl)acetate, was saponified and decarboxylated to yield II (R = 2-pyridyl).

ST benzyl phenyl ketone; pyridylmethyl phenyl ketone; benzene bisarylacetyl

IT 140-29-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation reaction of, with dimethyl terephthalate)

IT 100-20-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation reaction of, with ethyl pyridylacetate)

IT 120-61-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation reaction of, with phenylacetone nitrile)

IT 2739-98-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation reaction of, with terephthaloyl dichloride)

IT 3363-92-6P 64549-34-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

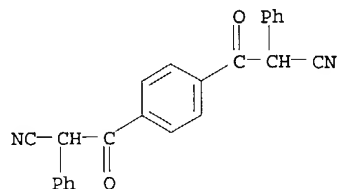
IT 64549-33-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, hydrolysis and decarboxylation of)

IT 64549-35-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, saponification and decarboxylation of)

IT 64549-33-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, hydrolysis and decarboxylation of)

RN 64549-33-3 HCAPLUS

CN 1,4-Benzenedipropanenitrile, .beta.,.beta.'-dioxo-.alpha.,.alpha.'-  
diphenyl- (9CI) (CA INDEX NAME)

L28 ANSWER 37 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1977:55276 HCAPLUS

DN 86:55276

ED Entered STN: 12 May 1984

TI Compositions comprising tetramic acid analogs of pulvinic acid for  
combating arthritis

IN Weinstock, Joseph

PA Smithkline Corp., USA

SO U.S., 12 pp. Division of U.S. 3,931,207.

CODEN: USXXAM

DT Patent

LA English

IC A61K031-40

NCL 424263000

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

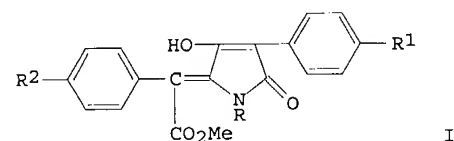
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3984559	A	19761005	US 1975-623226	19751017 <--
	US 3931207	A	19760106	US 1973-424581	19731214 <--
PRAI	US 1973-424581		19731214	<--	

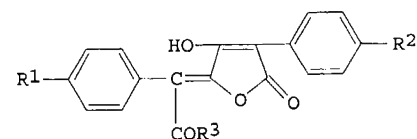
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3984559	IC	A61K031-40
	NCL	424263000

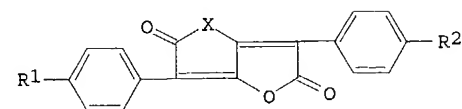
GI



I



II

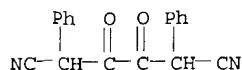


III

AB Tetramic acid derivs. I (R = 2-thiazolyl, 2-pyridyl, 5-chloro-2-pyridyl, 3-pyridyl, R1 = R2 = H; R = 2-thiazolyl, R1 = R2 = Cl; R = R2 = H, R1 = Me) were prepared by treating 4-R1C6H4CH2CN with (EtO2C)2, treating 4-R1C6H4CH(CN)CO2Et with 4-R2C6H4CH2CN, cyclizing 4-

Searched by Noble Jarrell

R1C6H4CH(CN)COCOCH(CN)C6H4R2-4 with acid, cyclizing II (R3 = OH) with  
 Ac2O, treating III (X = O) with RNH2, cyclizing II (R3 = NHR), and  
 methanolysis of III (X = NR).  
 ST tetramic acid benzylidene; benzylidenetetramic acid; thiazolytetramic  
 acid carboxybenzylidene; pyridyltetramic acid carboxybenzylidene;  
 arthritis tetramic acid  
 IT Arthritis  
 (tetramic acid derivs. in treatment of)  
 IT 140-29-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with ethyl oxalate)  
 IT 95-92-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with phenylacetoneitriles)  
 IT 10471-29-1P 26548-70-9P 38746-96-2P  
 38747-11-4P 38795-20-9P 55506-29-1P 55506-31-5P  
 55506-33-7P 55506-34-8P 61589-56-8P 61589-57-9P 61589-58-0P  
 61589-59-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization of)  
 IT 38558-87-1P 59522-36-0P 59522-41-7P 59522-46-2P 59522-49-5P  
 59522-52-0P 59522-56-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and methanolysis of)  
 IT 6273-79-6P 39992-21-7P 55506-38-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction of, with amines)  
 IT 38747-00-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with chlorophenylacetoneitrile)  
 IT 6362-63-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with phenylacetoneitriles)  
 IT 38747-12-5P 38747-15-8P 51780-73-5P 55506 32-6P  
 55506-35-9P 59522-37-1P 59522-42-8P 59522-47-3P 59522-53-1P  
 59522-57-5P 59522-60-0P 61589-54-6P 61589-55-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 500-98-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with benzoylformic acid)  
 IT 31603-77-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with cyanophenylpyruvate)  
 IT 140-53-4 2947-61-7 6775-77-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with oxalate)  
 IT 611-73-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetyl glycine)  
 IT 55506-37-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with pulvonic acid lactone)  
 IT 96-50-4 98-16-8 462-08-8 504-29-0 1072-98-6 5469-69-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with pulvonic acid lactone)  
 IT 10471-29-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation);  
 PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization of)  
 RN 10471-29-1 HCAPLUS  
 CN Hexanedinitrile, 3,4-dioxo-2,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



AN 1976:446362 HCAPLUS  
 DN 85:46362  
 ED Entered STN: 12 May 1984  
 TI Ester derivatives of pulvinic acid  
 IN Sutton, Blaine M.; Walz, Donald T.; Wilson, James W.  
 PA Smithkline Corp., USA  
 SO U.S., 7 pp. Division of U.S. 3,826,839.  
 CODEN: USXXAM

DT Patent

LA English

IC C07D

NCL 260343600

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

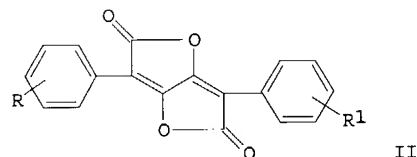
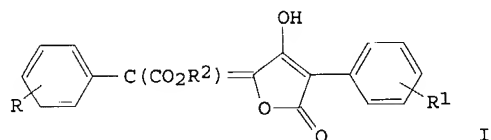
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3944571	A	19760316	US 1974-467367	19740506 <--
	US 3826839	A	19740730	US 1971-191051	19711020 <--
	CA 988851	A2	19760511	CA 1974-196994	19740408 <--
PRAI	US 1970-94974		19701203	<--	
	US 1971-191051		19711020	<--	
	CA 1971-127883		19711117	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3944571	IC	C07D
	NCL	260343600

GI



AB About 20 pulvinates I (R, R1 = H, p-Cl, m-Cl, p-MeO, p-F, m-MeO, p-EtO, etc.; R2 = Me, Et) were prepared by treating RC6H4CN with EtO2CCO2Et and condensation of RC6H4CH(CN)COCO2Et with R1C6H4CN to give RC6H4CH(CN)COCOCH(CN)C6H4R1, which was cyclized and the lactone II hydrolyzed. At 10-50 mg/kg I inhibited adjuvant induced arthritis in rats.

ST pulvinate antiarthritic; inflammation inhibitor pulvinate

IT Arthritis  
 (inhibitors, pulvinates)

IT Inflammation inhibitors  
 (pulvinates)

IT 38746-96-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis and cyclization of)

IT 5099-87-6 50886-27-6 59801-33-1 59801-34-2 59801-35-3 59801-36-4  
 59801-37-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis of)

IT 38747-06-7P 38747-07-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization and hydrolysis of)

IT 26548-70-9P 38747-10-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization of)

IT 10471-29-1P 38747-03-4P 38747-11-4P  
 38795-20-9P 50689-02-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis and cyclization of)

IT 6273-79-6P 20935-72-2P 22628-17-7P 38747-12-5P 38747-15-8P  
39992-21-7P 59801-31-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

IT 59801-30-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis or cyclization of)

IT 38746-75-7P 38746-76-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and oxidation of)

IT 6362-63-6P 38747-09-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with phenylacetonitrile)

IT 38747-00-1P 38747-05-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with phenylacetonitriles)

IT 481-59-4P 481-63-0P 481-64-1P 521-52-8P 22628-20-2P 22628-21-3P  
27394-71-4P 32883-73-1P 32883-77-5P 37542-20-4P 37542-21-5P  
37542-22-6P 37542-24-8P 37542-25-9P 38746-72-4P 38746-73-5P  
38746-74-6P 38746-77-9P 38746-78-0P 38746-79-1P 38746-80-4P  
38746-81-5P 38746-82-6P 38746-85-9P 38746-86-0P 38746-87-1P  
38746-88-2P 38746-89-3P 38746-90-6P 38746-91-7P 38747-14-7P  
59801-32-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 93-17-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with cyanophenylpyruvate and with diethyl oxalate)

IT 104-47-2 4439-02-5 19924-43-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diethyl oxalate)

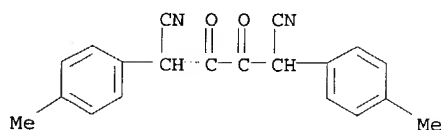
IT 140-29-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl oxalate)

IT 95-92-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylacetonitrile)

IT 104-47-2 140-53-4 2947-61-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl oxalate)

IT 38747-06-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization and hydrolysis of)

RN 38747-06-7 HCAPLUS  
CN Hexanedinitrile, 2,5-bis(4-methylphenyl)-3,4-dioxo- (9CI) (CA INDEX NAME)



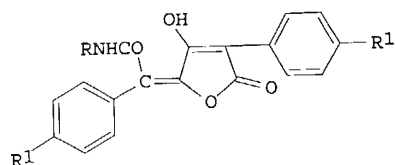
L28 ANSWER 39 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1976:421417 HCAPLUS  
DN 85:21417  
ED Entered STN: 12 May 1984  
TI Antiarthritic compositions comprising N-heterocyclic pulvinic acid amides  
IN Weinstock, Joseph  
PA Smithkline Corp., USA  
SO U.S., 9 pp. Division of U.S. 3,895,021.  
CODEN: USXXAM  
DT Patent  
LA English

IC A61K  
 NCL 424270000  
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 27

FAN.CNT 2		PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
PI	US	3947580		A	19760330	US 1975-562628	19750327 <--
	US	3895021		A	19750715	US 1973-393861	19730904 <--
	JP	50058067		A2	19750520	JP 1974-99429	19740828 <--
	JP	58017473		B4	19830407		
	GB	1434156		A	19760505	GB 1974-38260	19740902 <--
	BE	819495		A1	19750303	BE 1974-148174	19740903 <--
PRAI	US	1973-393861			19730904	<--	

CLASS		PATENT FAMILY CLASSIFICATION CODES	
PATENT NO.	CLASS		
US 3947580	IC NCL	A61K 424270000	

GI



I

AB Pulvinic acid amides I (R = 2-thiazolyl, 5-chloro-2-thiazolyl, 2-pyridyl, R1 = H; R = 2-thiazolyl, R1 = Cl, EtO), having anti-arthritic activity at 25 mg/kg (rats), were prepared. Thus, PhCH2CN condensed with (CO2Et)2 and NaOEt, the PhCH(CN)CO2Et treated with PhCH2CN in EtOH-NaOEt, the (NCCHPhCO)2 cyclized with AcOH-H2SO4, the pulvinic acid lactonized with Ac2O, and the lactone refluxed with 2-aminothiazole in CHCl3 to give I (R = 2-thiazolyl, R1 = H). Similarly prepared were 4-phenyl-, 4-chloro-4-methyl-, and 4,4'-diacetoxypulvinic acid lactones.

ST antiarthritic heterocyclyl pulvinic amide; diphenyldioxoadiponitrile cyclization; adiponitrile diphenyldioxo cyclization

IT Arthritis  
 (N-heterocycylpulvinic acid amides as inhibitors of)

IT 140-29-4 140-53-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with ethyl oxalate)

IT 95-92-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with phenylacetonitriles)

IT 38746-96-2 50689-10-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of)

IT 6362-63-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with phenylacetonitrile)

IT 10471-29-1P 38747-11-4P 38795-20-9P  
 51780-73-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization of)

IT 26548-70-9P 38747-01-2P 50689-13-9P 50689-14-0P 55032-45-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and lactonization of)

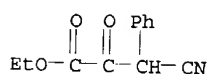
IT 38747-00-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with (chlorophenyl)acetonitrile)

IT 6273-79-6P 39992-21-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with heterocycyl amines)

IT 38558-83-7P 38747-12-5P 38747-15-8P 51780-75-7P 55506-29-1P  
 55506-30-4P 55506-31-5P 55506-32-6P 55506-33-7P 55506-34-8P  
 55506-35-9P

Searched by Noble Jarrell

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
IT 55506-38-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with aminothiazole)  
IT 31603-77-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl cyanophenylpyruvate)  
IT 504-29-0 1072-98-6 5469-69-2 55506-37-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with pulvinic acid lactone)  
IT 96-50-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with pulvinic acid lactones)  
IT 6362-63-6P  
RL: SPN (Synthetic preparation); SPN (Synthetic  
preparation); PREP (Preparation)  
(preparation and condensation with phenylacetonitrile)  
RN 6362-63-6 HCAPLUS  
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
INDEX NAME)



L28 ANSWER 40 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1976:421090 HCAPLUS  
DN 85:21090  
ED Entered STN: 12 May 1984  
TI Tetramic acid analogs of pulvinic acid  
IN Weinstock, Joseph  
PA Smithkline Corp., USA  
SO U.S., 13 pp.  
CODEN: USXXAM

DT Patent  
LA English  
IC C07D

NCL 260295500R

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3931207	A	19760106	US 1973-424581	19731214 <--
	US 3984559	A	19761005	US 1975-623226	19751017 <--
PRAI	US 1973-424581		19731214		<--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3931207	IC	C07D
	NCL	260295500R

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Seven tetramic acid derivs. I (R = thiazolyl, pyridyl, chloropyridyl, 3-F3CC6H4, H, R1 = H; R = thiazolyl, R1 = Cl), inhibitors of adjuvant-induced polyarthritis in rats at 50 mg/kg daily and antibacterials (no data), were prepared (for R .noteq. H) in 7 steps by condensation of 4-R1C6H4CH2CN with (EtO2C)2 via furanone II and tetramic acid lactone III. Ring cleavage of III gave I. To prepare I (R = R1 = H), BzCO2H was condensed with PhCH2CONHCH2CO2H to give anhydride IV which gave I (R = R1 = H) in 3 further steps. Seven further examples were given, but only the various intermediary compds. were characterized.

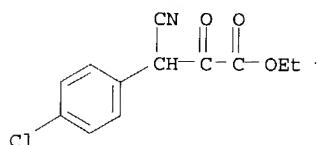
ST tetramic acid antiarthritic antibacterial; thiazolyltetramic acid pharmaceutical; pyridyltetramic acid pharmaceutical; fluorophenyltetramine acid pharmaceutical; acetonitrile condensation ethyl oxalate; adiponitrile hydrolysis cyclization; pulvinic acid amide cyclization

IT Bactericides, Disinfectants and Antiseptics  
Inflammation inhibitors



- ((carbomethoxyphenylmethylene)phenyltetramic acid derivs.)
- IT Lactones  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(of phenyltetramic acids, cleavage of, with sodium methoxide)
- IT Amides, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(of pulvinic acid, cyclization of, tetramic acid lactones by)
- IT Nitriles, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(phenylaceto, condensation with diethyl oxalate)
- IT 59522-41-7 59522-46-2 59522-49-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cleavage of, with sodium methoxide)
- IT 140-29-4 140-53-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with diethyl oxalate)
- IT 95-92-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation with phenylacetoneitriles)
- IT 59522-51-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of)
- IT 50689-13-9 50689-14-0 55032-45-6 59522-55-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydration of)
- IT 38746-96-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of)
- IT 50689-10-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis, dehydration, and acetylation of)
- IT 38558-87-1P 59522-36-0P 59522-52-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and cleavage with sodium methoxide)
- IT 38747-00-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and condensation with (chlorophenyl)acetonitrile)
- IT 6362-63-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and condensation with phenylacetoneitrile)
- IT 59522-35-9P 59522-40-6P 59522-45-1P 59522-48-4P 59534-90-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and cyclization of)
- IT 26548-70-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and dehydration of)
- IT 10471-29-1P 38747-11-4P 38795-20-9P  
51780-73-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)
- IT 59522-59-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and lactonization of)
- IT 59522-58-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and rearrangement of)
- IT 38558-83-7P 38747-12-5P 38747-15-8P 51780-75-7P 59522-37-1P  
59522-39-3P 59522-42-8P 59522-44-0P 59522-47-3P 59522-50-8P  
59522-53-1P 59522-54-2P 59522-57-5P 59522-60-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 38747-01-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation plus dehydration of)
- IT 6362-63-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with (chlorophenyl)acetonitrile)
- IT 611-73-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylacetyl glycine)
- IT 98-59-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with thiazolylpulvinic acid amide)  
 IT 39992-21-7 59522-43-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with aminothiazole)  
 IT 500-98-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with benzoylformic acid)  
 IT 6273-79-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with heterocyclamylamines)  
 IT 96-50-4 462-08-8 504-29-0 1072-98-6 2646-97-1 5469-69-2  
 55506-37-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with pulvinic acid lactones)  
 IT 59522-56-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ring cleavage of)  
 IT 38747-00-1P  
 RL: SPN (Synthetic preparation); SPN (Synthetic  
 preparation); PREP (Preparation)  
 (preparation and condensation with (chlorophenyl)acetonitrile)  
 RN 38747-00-1 HCAPLUS  
 CN Benzenepropanoic acid, 4-chloro-.beta.-cyano-.alpha.-oxo-, ethyl ester  
 (9CI) (CA INDEX NAME)



L28 ANSWER 41 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1975:609414 HCAPLUS  
 DN 83:209414  
 ED Entered STN: 12 May 1984  
 TI Anti-arthritic compositions comprising amide derivatives of pulvinic acid  
 IN Sutton, Blaine M.; Weinstock, Joseph  
 PA Smithkline Corp., USA  
 SO U.S., 5 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A61K  
 NCL 424279000  
 CC 63-6 (Pharmaceuticals)  
 Section cross-reference(s): 27, 25

FAN.CNT 1

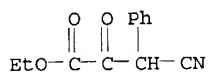
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3907997	A	19750923	US 1971-192588	19711026 <--
PRAI US 1971-192588		19711026 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3907997	IC	A61K
	NCL	424279000

GI For diagram(s), see printed CA Issue.  
 AB The antiarthritic pulvinic acid amide derivs., I where R1 and R2 = H, C1-4 alkyl, Cl, Br, and F were synthesized and formulations for their administration were described. Thus, 4,4'-dichloropulvinamide [57248-91-6] (whose synthesis was described) 50, Mg stearate 5, and lactose 350 mg/capsule were screened through a Number 40 mesh screen, mixed, and filled into Number 0 hard gelatin capsule.  
 ST pulvinamide deriv arthritis treatment  
 IT Arthritis  
 (pulvinamide derivs. for therapy of)  
 IT 6273-79-6P  
 RL: PREP (Preparation)  
 (prepn, and aminolysis of)  
 IT 38747-12-5P 39992-21-7P 50688-99-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)  
 (preparation and aminolysis of)  
 IT 31673-63-9P 57216-40-7P 57216-41-8P 57248-91-6P 57248-92-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and antiarthritic activity of)  
 IT 6362-63-6P 38747-00-1P 38747-05-6P  
 57248-93-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and aralkylation of)  
 IT 26548-70-9P 38747-01-2P 38747-07-8P 50689-13-9P 50689-14-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and cyclization of)  
 IT 10471-29-1P 38747-06-7P 38747-11-4P  
 38795-20-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and hydrolysis of)  
 IT 140-29-4 140-53-4 2947-60-6 2947-61-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diethyl oxalate)  
 IT 95-92-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetoneitriles)  
 IT 6362-63-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and aralkylation of)  
 RN 6362-63-6 HCAPLUS  
 CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
 INDEX NAME)



L28 ANSWER 42 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1975:593065 HCAPLUS  
 DN 83:193065  
 ED Entered STN: 12 May 1984  
 TI Antiarthritic phenylvulpinic acid derivatives  
 IN Sutton, Blaine M.  
 PA Smithkline Corp., USA  
 SO U.S., 5 pp. Division of U.S. 3,780,065.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC A61K  
 NCL 424279000  
 CC 27-6 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 23, 25

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3896234	A	19750722	US 1973-393235	19730830 <--
	US 3780065	A	19731218	US 1972-279597	19720810 <--
PRAI	US 1971-188555		19711013	<--	
	US 1972-279597		19720810	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3896234	IC	A61K
	NCL	424279000

GI For diagram(s), see printed CA Issue.

AB The title compds. I (R = 3-Ph, 4-Ph, R1 = H; R = H, R1 = 3-Ph, 4-Ph), which inhibited adjuvant arthritis in rats at 20-5 mg/kg, were prepared Thus, condensation of PhCH2CN and (CO2Et)2 gave PhCH(CN)CO2Et, which condensed with PhC6H4CH2Cl to give PhCH(CN)COCOCH(CN)C6H4Ph (II). Hydrolysis and lactonization of II gave the phenylpulpinic acid lactones III, which were hydrolyzed in KOH-MeOH to give I.  
 ST phenylvulpinic acid arthritis inhibitor; dioxadiponitrile hydrolysis cyclization

IT Arthritis  
(phenylvulpinates in treatment of)

IT 51780-76-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction of, with ethyl 3-cyano-3-phenylpyruvate)

IT 31603-77-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction with ethyl 3-cyano-3-phenylpyruvate)

IT 140-29-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction with ethyl oxalate)

IT 95-92-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction with phenylacetoneitrile)

IT 51780-77-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of)

IT 51780-88-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and antiarthritic activity of)

IT 6362-63-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and condensation reaction with biphenylacetoneitriles)

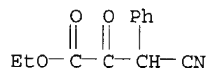
IT 51780-73-5P 51780-75-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

IT 55506-39-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and lactonization of)

IT 6362-63-6P  
RL: SPN (Synthetic preparation); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and condensation reaction with biphenylacetoneitriles)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 43 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1975:409762 HCAPLUS

DN 83:9762

ED Entered STN: 12 May 1984

TI .alpha..beta.-Unsaturated esters of vulpinic acid

IN Sutton, Blaine M.

PA Smithkline Corp.

SO U.S., 6 pp. Division of U.S. 3,749,740 (CA 79: 91979w).

CODEN: USXXAM

DT Patent

LA English

IC A61K

NCL 424285000

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3865947	A	19750211	US 1973-357982	19730507 <--
	US 3749740	A	19730731	US 1972-276020	19720728 <--
PRAI	US 1971-150209		19710604	<--	
	US 1972-276020		19720728	<--	

CLASS

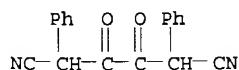
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3865947	IC	A61K
	NCL	424285000

GI For diagram(s), see printed CA Issue.

AB The vulpinic acid derivs. I (R, R1 = H, 4-MeO; R = R1 = H, 4-Cl, 4-F, 3,4,5-(MeO)C6H3; R2 = H, CH2:CHCO, CH2:CMeCO) were prepared Thus, PhCH2CN was treated with EtO2CCO2Et and the resulting PhCH(CN)COCO2Et treated with

PhCH<sub>2</sub>CN to give PhCH(CN)COCOCH(CN)Ph which was cyclized to pulvinic acid lactone(II). II and MeOH gave I (R = R<sub>1</sub> = H, R<sub>2</sub> = H), which with CH<sub>2</sub>:CHCOCl gave I (R = R<sub>1</sub> = H, R<sub>2</sub> = COCH:CH<sub>2</sub>). At 10-150 mg I were antiarthritic.

- ST vulpinic acid acryloyl antiarthritic; antiarthritic acryloyl vulpinate; adiponitrile dioxo diphenyl cyclization; cyclization diphenyldioxoadiponitrile; pulvinic acid lactone
- IT Arthritis  
(vulpinic acid derivative in treatment of)
- IT 6273-79-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of)
- IT 521-52-8P 37542-25-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and acylation of)
- IT 10471-29-1P 26548-70-9P 38731-08-7P 38747-01-2P  
38747-03-4P 38747-06-7P 38747-07-8P  
38795-20-9P 50689-02-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)
- IT 481-64-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and esterification of)
- IT 22628-17-7P 38589-34-3P 39992-21-7P 50886-27-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)
- IT 38746-87-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with methanol)
- IT 38747-00-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with p-chlorophenylacetonitrile)
- IT 6362-63-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with phenylacetonitrile)
- IT 22628-20-2P 37542-24-8P 38746-88-2P 38746-90-6P 50688-92-1P  
50688-93-2P 50688-95-4P 50688-98-7P 50689-05-9P 55697-19-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 104-47-2 140-29-4 140-53-4 459-22-3 2947-61-7 13338-63-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diethyl oxalate)
- IT 95-92-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylacetonitrile)
- IT 814-68-6 920-46-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with vulpinic acids)
- IT 10471-29-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)
- RN 10471-29-1 HCAPLUS
- CN Hexanedinitrile, 3,4-dioxo-2,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 44 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1974:520257 HCAPLUS  
DN 81:120257  
ED Entered STN: 12 May 1984  
TI Substituted 2,5-diphenyl-3,4,6-trihydroxy-.DELTA.2,4-hexadienoic acid lactones (1,4) in the treatment of arthritis  
IN Sutton, Blaine M.

PA Smithkline Corp.  
 SO U.S., 4 pp. Division of U. S. 3,772,341 (CA 80;133047u).  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A61K  
 NCL 424279000  
 CC 25-18 (Noncondensed Aromatic Compounds)  
 Section cross-reference(s): 63

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3821398	A	19740628	US 1973-383643	19730730 <--
PRAI US 1970-148890		19700601 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3821398	IC NCL	A61K 424279000

GI For diagram(s), see printed CA Issue.

AB Title lactones (I; R = CH<sub>2</sub>OH, R<sub>1</sub> = Ph or substituted phenyl), useful as inhibitors for adjuvant-induced polyarthritis in rats, were prepared by reduction of pulvinic acids I (R = CO<sub>2</sub>H) (II) with B<sub>2</sub>H<sub>6</sub> in THF. II were prepared in several steps from R<sub>1</sub>CH<sub>2</sub>CN. Thus, condensation of PhCH<sub>2</sub>CN with (CO<sub>2</sub>Et)<sub>2</sub> in THF containing EtONa gave PhCH(CN)COCO<sub>2</sub> Et, which with PhCH<sub>2</sub>CN gave PhCH(CN)COCOCHPhCN. Hydrolysis of the latter with aqueous HOAc-H<sub>2</sub>SO<sub>4</sub> gave II (R<sub>1</sub> = Ph).

ST lactone hydroxyphenylhexadienoic acid arthritis; hexadienoic acid hydroxyphenyl lactone; phenylhexadienoic acid hydroxy lactone; pulvinic acid

IT Arthritis

(adjuvant-induced poly-, hydroxyphenyl hexadienoic lactones effect on)

IT 20935-70-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis of)

IT 38747-00-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with (chlorophenyl)acetonitrile)

IT 38747-09-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with (dimethoxyphenyl)acetonitrile)

IT 6362-63-6P 41339-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with phenylacetonitrile)

IT 38747-05-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with tolylacetonitrile)

IT 10471-29-1P 38747-03-4P 38795-20-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and hydrolysis of)

IT 38747-10-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reduction of)

IT 26548-70-9P 38747-01-2P 38747-07-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reduction of)

IT 38747-02-3P 38747-06-7P 53587-70-5P 53587-71-6P  
 53658-64-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 93-17-4 104-47-2 140-29-4 140-53-4 1529-41-5 2947-61-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diethyl oxalate)

IT 95-92-1

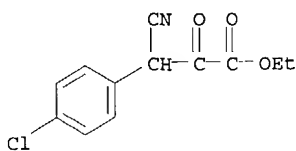
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetonitrile)

IT 38747-00-1P

RL: SPN (Synthetic preparation); PREP (Preparation);  
 PREP (Preparation)  
 (preparation and condensation with (chlorophenyl)acetonitrile)

RN 38747-00-1 HCAPLUS

CN Benzenepropanoic acid, 4-chloro-.beta.-cyano-.alpha.-oxo-, ethyl ester  
 (9CI) (CA INDEX NAME)



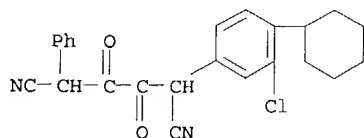
L28 ANSWER 45 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1974:505256 HCAPLUS  
 DN 81:105256  
 ED Entered STN: 12 May 1984  
 TI 4-Cyclohexylvulpinic acid derivatives in the treatment of arthritis  
 IN Sutton, Blaine M.  
 PA Smithkline Corp.  
 SO U.S., 4 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC A61K  
 NCL 424279000  
 CC 27-6 (Heterocyclic Compounds (One Hetero Atom))  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3821397	A	19740628	US 1973-357762	19730507 <--
	US 3752829	A	19730814	US 1972-282534	19720821 <--
PRAI	US 1971-188439		19711013		<--
	US 1972-282534		19720821		<--

## CLASS

	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
	US 3821397	IC	A61K
		NCL	424279000
GI	For diagram(s), see printed CA Issue.		
AB	PhCH <sub>2</sub> CN was treated with EtO <sub>2</sub> CCO <sub>2</sub> Et and the resulting PhCH(CN)COCO <sub>2</sub> Et treated with 3-chloro-4-cyclohexylphenylacetonitrile and the product cyclized with HOAc to give 3'-chloro-4'-cyclohexylpulpinic acid, which was cyclized and the resulting 3'-chloro-4'-cyclohexylpulpinic acid lactone cleaved with HCl to give the vulpinic oxides I and II. I and II are antiarthritic at 16 mg/kg in rats.		
ST	vulpinic acid cyclohexyl antiarthritic; antiarthritic cyclohexylvulpinic acid; pulvinic acid chloro cyclohexyl		
IT	Arthritis		
	(adjuvant, cyclohexylvulpinic acids as inhibitors for)		
IT	50548-55-5P		
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cleavage of)		
IT	50548-53-3P 50548-54-4P		
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of)		
IT	6362-63-6P		
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with 3-chloro-4-cyclohexylphenylacetonitrile)		
IT	50513-91-2P 50548-56-6P		
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)		
IT	26961-79-5		
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ethyl 3-cyano-3-phenylpyruvate)		
IT	140-29-4		
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ethyl oxalate)		
IT	95-92-1		
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phenylacetonitrile)		
IT	50548-53-3P		
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of)		
RN	50548-53-3 HCAPLUS		

CN Hexanedinitrile, 2-(3-chloro-4-cyclohexylphenyl)-3,4-dioxo-5-phenyl- (9CI)  
(CA INDEX NAME)



L28 ANSWER 46 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1974:491367 HCAPLUS  
DN 81:91367  
ED Entered STN: 12 May 1984  
TI Pyridyl ketipate lactones and derivatives in treating arthritis  
IN Sutton, Blaine M.  
PA Smithkline Corp.  
SO U.S., 4 pp. Divison of U.S. 3,714,1733 (CA 78;111148j).  
CODEN: USXXAM

DT Patent  
LA English  
IC A61K  
NCL 424266000  
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 28

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3818092	A	19740618	US 1972-287381	19720908 <--
	US 3714173	A	19730130	US 1971-160190	19710706 <--
PRAI	US 1971-160190		19710706	<--	

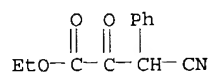
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3818092	IC	A61K
	NCL	424266000

GI For diagram(s), see printed CA Issue.  
AB PhCH<sub>2</sub>CN was treated with EtO<sub>2</sub>CCO<sub>2</sub>Et and the resulting Ph-CH(CN)COCO<sub>2</sub>Et treated with 3-pyridylacetonitrile to give 2-phenyl-5-(3-pyridyl)-3,4-dioxoadiponitrile, which was cyclized with H<sub>2</sub>SO<sub>4</sub> and the resulting ketipic acid dilactone I treated with Ac<sub>2</sub>O to give the ketipate lactone II (R = R<sub>1</sub> = H). II (R = H, R<sub>1</sub> = Cl, F3C) were similarly prepared II (R = R<sub>1</sub> = H) and acyl chlorides gave II (R = H<sub>2</sub>C:CHCO, H<sub>2</sub>C:CMeCO, PhCH:CH-CO; R<sub>1</sub> = H). At 25 mg/kg II inhibited adjuvant arthritis in rats.  
ST ketipate lactone pyridyl antiarthritic; antiarthritic pyridylketipate lactone; cyclization pyridyldioxoadiponitrile; adiponitrile dioxo pyridyl cyclization  
IT Arthritis  
(adjuvant, inhibition by pyridylketipate lactones)  
IT 6362-63-6P 38747-00-1P 40517-14-4P  
40517-16-6P 40517-17-7P 40517-18-8P 40517-19-9P 40517-22-4P  
40517-23-5P 40575-04-0P 53353-07-4P 53353-09-6P  
53353-10-9P 53353-56-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
IT 140-53-4 2338-75-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with diethyl oxalate)  
IT 6443-85-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl 3-cyano-3-phenylpyruvate)  
IT 140-29-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl oxalate)  
IT 102-92-1 814-68-6 920-46-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with methyl 2-phenyl-5-(3-pyridyl)ketipate lactone)  
IT 95-92-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylacetonitriles)  
IT 6362-63-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)



RN 6362-63-6 HCAPLUS  
 CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
 INDEX NAME)



L28 ANSWER 47 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1974:491365 HCAPLUS

DN 81:91365

ED Entered STN: 12 May 1984

TI Pyridyl ketipate lactones and derivatives

IN Sutton, Blaine M.

PA Smithkline Corp.

SO U.S., 3 pp.

CODEN: USXXAM

DT Patent

LA English

IC C07D

NCL 260295000R

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 28

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3816440	A	19740611	US 1973-393234	19730830 <--
	US 3714173	A	19730130	US 1971-160190	19710706 <--
	US 3781295	A	19731225	US 1972-287189	19720907 <--
PRAI	US 1971-160190		19710706	<--	
	US 1972-287189		19720907	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3816440	IC	C07D
	NCL	260295000R

GI For diagram(s), see printed CA Issue.

AB Ph-CH<sub>2</sub>CN was treated with EtO<sub>2</sub>CCO<sub>2</sub>Et and the resulting PhCH-(CN)COCO<sub>2</sub>Et treated with 3-pyridylacetonitrile to give 2-phenyl-5-(3-pyridyl)-3,4-dioxoadiponitrile, which was cyclized with AcOH and H<sub>2</sub>SO<sub>4</sub> and the resulting ketipic acid dilactone I treated with Ac<sub>2</sub>O to give the ketipate lactone II (R = R<sub>1</sub> = H). II (R = H, R<sub>1</sub> = Cl, CF<sub>3</sub>) were similarly prepared II (R = R<sub>1</sub> = H) and acyl chlorides gave II (R = H<sub>2</sub>C:CHCO, H<sub>2</sub>C:CMeCO, PhCH:CHCO; R<sub>1</sub> = H). At 25 mg/kg II inhibited adjuvant arthritis in rats.

ST ketipate lactone pyridyl antiarthritic; antiarthritic pyridylketipate lactone; cyclization pyridyldioxoadiponitrile; adiponitrile dioxo pyridyl cyclization

IT Arthritis

(pyridylketipate lactones in treatment of)

IT 6362-63-6P 38747-00-1P 40517-14-4P  
 40517-16-6P 40517-17-7P 40517-18-8P 40517-19-9P 40517-22-4P  
 40517-23-5P 40575-04-0P 53353-07-4P 53353-08-5P  
 53353-09-6P 53353-10-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 102-92-1 814-68-6 920-46-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with 2-phenyl-5-(3-pyridyl)ketipate lactone)

IT 140-29-4 140-53-4 2338-75-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diethyl oxalate)

IT 6443-85-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with ethyl 3-cyano-3-phenylpyruvate)

IT 95-92-1

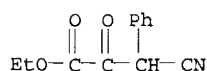
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetonitriles)

IT 6362-63-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
 INDEX NAME)



L28 ANSWER 48 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1974:133047 HCAPLUS  
 DN 80:133047  
 ED Entered STN: 12 May 1984  
 TI Substituted 2,5-diphenyl-3,4,6-trihydroxy-.DELTA.2,4-hexadienoic acid  
 lactones (1,4)  
 IN Sutton, Blaine M.  
 PA Smith Kline French Laboratories  
 SO U.S., 3 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07D  
 NCL 260343600  
 CC 25-17 (Noncondensed Aromatic Compounds)  
 Section cross-reference(s): 27

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3772341	A	19731113	US 1971-148890	19710601 <--
PRAI US 1971-148890		19710601 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3772341	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.

AB The title compds. (I; R, R1 = H, Me MeO, CF3, halo) having antiarthritic activity at 25 mg/kg-day in rats were prepared by diborane reduction of pulvinic acid derivs. Thus, a mixture of PhCH2CN and Et oxalate was refluxed in NaOEt solution to give PhCH(CN)COCO2Et, which was refluxed with PhCH2CN in NaOEt solution to give 2,5-diphenyl-3,4-dioxoadiponitrile (II). A mixture of II in H2O, HOAc, and concentrated H2SO4 was refluxed 1 hr to give pulvinic acid, which was reduced with B2H6 in THF to give the lactone (I; R = R1 = H). Similarly prepared were 7 I including a trimethoxyphenyl derivative

ST antiarthritic diaryltri-hydroxyhexadienoic lactone; furanone hydroxy diphenyl antiarthritic

IT Arthritis

(diaryltri-hydroxyhexadienoic lactones in treatment of)

IT 10471-29-1P 20935-70-0P 38747-03-4P

38747-06-7P 38795-20-9P 50689-02-6P

52387-78-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

IT 38747-00-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction with (chlorophenyl)acetonitrile)

IT 38747-09-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction with (dimethoxyphenyl)acetonitrile)

IT 50689-01-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction with (fluorophenyl)acetonitrile)

IT 41339-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction with (methoxyphenyl)acetonitrile)

IT 52387-79-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction with (methylphenyl)acetonitrile)

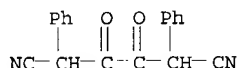
IT 6362-63-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

Searched by Noble Jarrell

(preparation and reaction with phenylacetonitrile)  
 IT 26548-70-9P 38747-01-2P 38747-07-8P 38747-10-3P 50688-96-5P  
 50688-97-6P 50689-03-7P 50689-07-1P 50689-08-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reduction of)  
 IT 93-17-4 104-47-2 140-29-4 140-53-4 459-22-3 2947-61-7  
 13338-63-1  
 RL: PROC (Process)  
 (substitution of, with Et oxalate)  
 IT 10471-29-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and hydrolysis of)  
 RN 10471-29-1 HCAPLUS  
 CN Hexanedinitrile, 3,4-dioxo-2,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 49 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1974:95710 HCAPLUS

DN 80:95710

ED Entered STN: 12 May 1984

TI Thiopulvinic acid derivatives

IN Weinstock, Joseph

PA Smithkline Corp.

SO U.S., 4 pp.

CODEN: USXXAM

DT Patent

LA English

IC C07C

NCL 260343600

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3780064	A	19731218	US 1972-267762	19720630 <--
	US 3852462	A	19741203	US 1973-393236	19730830 <--
PRAI	US 1972-267762		19720630	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3780064	IC	C07C
	NCL	260343600

GI For diagram(s), see printed CA Issue.

AB The thiopulvinic acids I (R = Me, Ph, PhCH<sub>2</sub>, R<sub>1</sub> = R<sub>2</sub> = H; R = Me, R<sub>1</sub> = R<sub>2</sub> = Cl; R = Me, R<sub>1</sub> = Ph, R<sub>2</sub> = H) were prepared. Thus, PhCH<sub>2</sub>CN was treated with EtO<sub>2</sub>CCO<sub>2</sub>Et and the resulting PhCH(CN)COCO<sub>2</sub>Et treated with PhCH<sub>2</sub>CN to give PhCH(CN)COCOCH(CN)Ph, which was treated with HOAc and the resulting pulvinic acid cyclized to give pulvinic acid lactone. The lactone and MeSH gave I (R = Me, R<sub>1</sub> = R<sub>2</sub> = H). At 25 mg/kg I inhibited adjuvant arthritis in rats induced by Mycobacterium butyricum.

ST pulvinic acid thio antiarthritic; antiarthritic thiopulvinic acid

IT Arthritis

(thiopulvinic acids in treatment of)

IT 6273-79-6P 6362-63-6P 10471-29-1P 26548-70-9P  
 38747-00-1P 38795-20-9P 39992-21-7P  
 51780-73-5P 51780-75-7P 51780-78-0P 51796-34-0P  
 51796-35-1P 51796-36-2P 51796-37-3P 51796-38-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 31603-77-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Et cyanophenylpyruvate)

IT 140-29-4 140-53-4

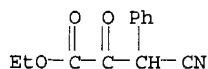
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Et oxalate)

IT 95-92-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetonitrile)

IT 74-93-1 100-53-8 108-98-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with pulvinic acid lactone)  
 IT 6362-63-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 6362-63-6 HCAPLUS  
 CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
 INDEX NAME)



L28 ANSWER 50 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1974:82677 HCAPLUS  
 DN 80:82677  
 ED Entered STN: 12 May 1984  
 TI Pyridyl ketipate lactones and derivatives  
 IN Sutton, Blaine M.  
 PA Smithkline Corp.  
 SO U.S., 3 pp. Division of U.S. 3,714,173 (CA 78;111148j).  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07D  
 NCL 260295000R  
 CC 27-17 (Heterocyclic Compounds (One Hetero Atom))  
 FAN.CNT 4

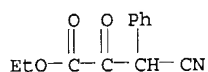
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3781295	A	19731225	US 1972-287189	19720907 <--
	US 3714173	A	19730130	US 1971-160190	19710706 <--
	US 3816440	A	19740611	US 1973-393234	19730830 <--
PRAI	US 1971-160190		19710706	<--	
	US 1972-287189		19720907	<--	

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3781295	IC	C07D
	NCL	260295000R

GI For diagram(s), see printed CA Issue.  
 AB The pyridyl ketipate lactones I (R = H, CH<sub>2</sub>:CHCO, CH<sub>2</sub>:CMeCO, PhCH:CHCO; R<sub>1</sub> = H, Cl; R<sub>2</sub> = Me, Et) were prepared Thus, PhCH<sub>2</sub>CN was treated with the EtO<sub>2</sub>CCO<sub>2</sub>Et and NaOEt and the resulting PhCH(CN)COCO<sub>2</sub>Et treated with 3-pyridylacetoneitrile to give 2-phenyl-5-(3-pyridyl)-3,4-dioxoadiponitrile which was treated with concentrated H<sub>2</sub>SO<sub>4</sub> to give I (R = R<sub>1</sub> = R<sub>2</sub> = H). The acid was esterified and then acylated with CH<sub>2</sub>:CHCOCl to give I (R = CH<sub>2</sub>:CHCO, R<sub>1</sub> = H, R<sub>2</sub> = Me). At 25 mg/kg I inhibited adjuvant arthritis produced by Mycobacterium butyricum in rats.  
 ST ketipate lactone pyridyl antiarthritic; antiarthritic pyridyl ketipate lactone; analgesic pyridyl ketipate lactone; antipyretic pyridyl ketipate lactone  
 IT Arthritis  
 (inhibitors of, pyridylketipate lactones)  
 IT Analgesics  
 Antipyretics  
 (pyridylketipate lactones)  
 IT 75-05-8, reactions 140-53-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with Et oxalate)  
 IT 95-92-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with phenylacetoneitriles)  
 IT 6362-63-6P 38747-00-1P 40517-14-4P  
 40517-15-5P 40517-16-6P 40517-17-7P 40517-18-8P 40517-19-9P  
 40517-21-3P 40517-22-4P 40517-23-5P 40575-04-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 6443-85-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Et 3-cyano-3-phenylpyruvate)  
 IT 814-68-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Me 2-phenyl-5-(3-pyridyl) ketipate lactone)  
 IT 102-92-1 920-46-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with Me 2-phenyl-5-(3-pyridyl)ketipate lactone)  
 IT 6362-63-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 6362-63-6 HCAPLUS  
 CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
 INDEX NAME)



L28 ANSWER 51 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1974:82624 HCAPLUS

DN 80:82624

ED Entered STN: 12 May 1984

TI Phenylvulpinic acid derivatives

IN Sutton, Blaine M.

PA Smithkline Corp.

SO U.S., 4 pp.

CODEN: USXXAM

DT Patent

LA English

IC C07D

NCL 260343600

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3780065	A	19731218	US 1972-279597	19720810 <--
	US 3896234	A	19750722	US 1973-393235	19730830 <--
PRAI	US 1971-188555		19711013	<--	
	US 1972-279597		19720810	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3780065	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.

AB Antiinflammatory 4-phenylvulpinic acid (I, R = H) was prepared by treating PhCH<sub>2</sub>CN with (CO<sub>2</sub>Et)<sub>2</sub> and treating the PhCH(CN)COCO<sub>2</sub>Et with p-PhC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CN to give PhCH(CN)COCOCH(CN)C<sub>6</sub>H<sub>4</sub>Ph-p. Acid cyclization yielded 4'-phenylpulvinic acid and then its lactone, which was cleaved with base and esterified with MeOH to give I (R = H). Treatment of I (R = H) with acid chlorides gave I (R = CH<sub>2</sub>:CHCO, CH<sub>2</sub>:CMeCO, Me<sub>2</sub>C:CHCO, MeCH:CHCO, PhCH:CHCO). 3-Phenylvulpinic acid was similarly prepared

ST antiinflammatory phenylvulpinic acid; vulpinic acid phenyl antiinflammatory

IT Inflammation inhibitors  
 (phenylvulpinic acids)

IT	6362-63-6P	51780-16-6P	51780-17-7P	51780-18-8P	51780-19-9P
	51780-20-2P	51780-22-4P	51780-73-5P	51780-74-6P	
	51780-75-7P	51780-77-9P	51780-78-0P	51780-79-1P	51780-80-4P
	51780-81-5P	51780-82-6P	51780-83-7P	51780-84-8P	51780-86-0P
	51780-87-1P	51780-88-2P			

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 51780-21-3 51780-85-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with acyl chlorides)

IT 31603-77-7 51780-76-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with cyano(phenyl)pyruvate)

IT 140-29-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with oxalate)

IT 95-92-1

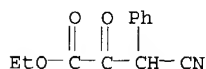
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetonitrile)

IT 6362-63-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
INDEX NAME)



L28 ANSWER 52 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:515428 HCAPLUS

DN 79:115428

ED Entered STN: 12 May 1984

TI 4-Cyclohexylvulpinic acid derivatives

IN Sutton, Blaine M.

PA Smith Kline and French Laboratories

SO U.S., 3 pp.

CODEN: USXXAM

DT Patent

LA English

IC C07D

NCL 260343600

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3752829	A	19730814	US 1972-282534	19720821 <--
	US 3821397	A	19740628	US 1973-357762	19730507 <--
PRAI	US 1971-188439		19711013		<--
	US 1972-282534		19720821		<--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3752829	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.

AB PhCH<sub>2</sub>CN was treated with (CO<sub>2</sub>Et)<sub>2</sub> and the resulting Et 2-cyano-3-phenylpyruvate treated with 3-chloro-4-cyclohexylphenylacetone to give 2-(3-chloro-4-cyclohexylphenyl)-5-phenyl-3,4-dioxoadiponitrile, which with H<sub>2</sub>O, HOAc, and concentrated H<sub>2</sub>SO<sub>4</sub> gave 3'-chloro-4'-cyclohexylvulpinic acid. The acid was converted to 3'-chloro-4'-cyclohexylvulpinic acid lactone, which with HCl in MeOH gave 3'-chloro-4'-cyclohexylvulpinic acid (I) and 3-chloro-4-cyclohexylvulpinic acid (II). At 16 mg/kg (oral, rat) the Me esters of I and II inhibited development of adjuvant arthritis.

ST vulpinic acid cyclohexyl antiarthritic; antiarthritic chlorocyclohexylvulpinic acid

IT Arthritis  
(inhibitor of, cyclohexylvulpinic acids)

IT 6362-63-6P 50513-91-2P 50548-53-3P 50548-54-4P  
50548-55-5P 50548-56-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 26961-79-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl 3-cyano-3-phenylpyruvate)

IT 140-29-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with ethyl oxylate)

IT 95-92-1

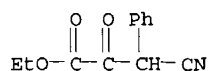
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylacetone nitrile)

IT 6362-63-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA  
INDEX NAME)



L28 ANSWER 53 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1973:491979 HCAPLUS  
 DN 79:91979  
 ED Entered STN: 12 May 1984  
 TI .alpha.,.beta.-Unsaturated esters of vulpinic acid  
 IN Sutton, Blain M.  
 PA Smith Kline and French Laboratories  
 SO U.S., 4 pp.  
 CODEN: USXXAM

DT Patent

LA English

IC C07D

NCL 260343600

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3749740	A	19730731	US 1972-276020	19720728 <--
US 3865947	A	19750211	US 1973-357982	19730507 <--
PRAI US 1971-150209		19710604	<--	
US 1972-276020		19720728	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3749740	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.

AB Vulpinic acid esters (I, R = CH<sub>2</sub>:CHCO, CH<sub>2</sub>:CHMeCO, MeCH:CHCO, Me<sub>2</sub>C:CHCO, PhCH:CHCO; R<sub>1</sub>, R<sub>2</sub> = e.g., H, Cl, MeO, Me), useful for treating arthritis were prepared. Thus, PhCH<sub>2</sub>CN was treated with (CO<sub>2</sub>Et)<sub>2</sub> to give [PhCH(CN)CO]<sub>2</sub> which on reaction with Ac<sub>2</sub>O followed by refluxing in MeOH/HCl gave vulpinic acid. Acylation of this with CH<sub>2</sub>:CHCOCl gave I (R = CH<sub>2</sub>:CHCO, R<sub>1</sub> = R<sub>2</sub> = H).

ST vulpinic acid ester arthritis

IT Arthritis

(vulpinic acid esters in treatment of)

IT 481-64-1P 521-52-8P 6273-79-6P 6362-63-6P  
 10471-29-1P 22628-17-7P 22628-20-2P 26548-70-9P  
 37542-22-6P 37542-23-7P 37542-24-8P 37542-25-9P 38589-34-3P  
 38731-08-7P 38746-87-1P 38746-88-2P 38746-90-6P 38747-00-1P  
 38747-01-2P 38747-03-4P 38747-05-6P  
 38747-06-7P 38747-07-8P 38747-11-4P 38747-12-5P  
 38795-20-9P 39992-21-7P 41339-41-7P 50674-92-5P  
 50688-92-1P 50688-93-2P 50688-94-3P 50688-95-4P 50688-96-5P  
 50688-97-6P 50688-98-7P 50688-99-8P 50689-00-4P 50689-01-5P  
 50689-02-6P 50689-03-7P 50689-04-8P 50689-05-9P  
 50689-06-0P 50689-07-1P 50689-08-2P 50689-09-3P  
 50689-10-6P 50689-11-7P 50689-12-8P 50689-13-9P  
 50689-14-0P 50689-15-1P 50689-16-2P 50886-27-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 104-47-2 140-29-4 140-53-4 459-22-3 2947-61-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diethyl oxalate)

IT 13338-63-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with ethyl cyanophenylpyruvate)

IT 95-92-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetoneitrile)

IT 102-92-1 814-68-6 920-46-7 10487-71-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with vulpinic acid)

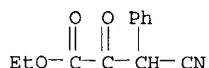
IT 6362-63-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA

## INDEX NAME)



L28 ANSWER 54 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1973:111148 HCAPLUS  
 DN 78:111148  
 ED Entered STN: 12 May 1984  
 TI Pyridyl ketipate lactones and derivatives  
 IN Sutton, Blaine M.  
 PA Smith Kline and French Laboratories  
 SO U.S., 3 pp.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC C07D

NCL 260295000R

CC 27-17 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3714173	A	19730130	US 1971-160190	19710706 <--
	US 3781295	A	19731225	US 1972-287189	19720907 <--
	US 3818092	A	19740618	US 1972-287381	19720908 <--
	US 3816440	A	19740611	US 1973-393234	19730830 <--
PRAI	US 1971-160190		19710706 <--		
	US 1972-287189		19720907 <--		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3714173	IC	C07D
	NCL	260295000R

GI For diagram(s), see printed CA Issue.

AB p-RC6H4CH2CN (R = H, Cl) and (CO2Et)2 reacted in EtOH containing NaOEt to give p-RC6H4CH(CN)COCO2Et, which condensed with 3-pyridylacetonitrile (R1CH2CN) in diglyme in the presence of NaH to yield p-RC6H4CH(CN)COCOCHR1CN. The latter compds. were treated with H2SO4 in HOAc give the ketipic acid lactones I (R = H, Cl, R2 = H), which were refluxed in Ac2O and then treated with MeOH containing KOH to give I (R = H, Cl = R2 = Me), which possessed anti-anthritic activity. I (R = H, R2 = Me) was treated with CH2:-CHCOCl, CH2:CMCOCl, and PhCH:CHCOCl in CHCl3 containing pyridine to yield ketipic lactones II (r = CH2:CHCO, CH2CMCO, PhCH:CHCO).

ST ketipic acid lactone antiarthritic; pyridine ketipic lactone antiarthritic

IT Arthritis

(Me pyridylketipate lactone effect on)

IT 6443-85-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with cyanopyruvate derivs.)

IT 40517-16-6P 40517-22-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and antiarthritic activity of)

IT 6362-63-6P 38747-00-1P 40517-14-4P

40517-15-5P 40517-17-7P 40517-18-8P 40517-19-9P 40517-21-3P  
 40517-23-5P 40575-04-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 140-29-4 140-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diethyl oxalate)

IT 95-92-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with phenylacetonitrile derivs.)

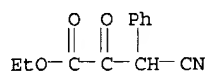
IT 6362-63-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)





L28 ANSWER 55 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1972:140776 HCAPLUS  
 DN 76:140776  
 ED Entered STN: 12 May 1984  
 TI Antibacterial and antiprotozoal 3-(5-nitro-2-furyl)isoxazoline derivatives  
 IN Minami, Shinsaku; Matsumoto, Junichi; Shimizu, Masanao; Takase, Yoshiyuki  
 PA Dainippon Pharmaceutical Co., Ltd.  
 SO U.S., 10 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC C07D  
 NCL 260247500R  
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3631169	A	19711228	US 1966-581192	19660922 <--
PRAI US 1966-581192		19660922 <--		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3631169	IC	C07D
	NCL	260247500R

GI For diagram(s), see printed CA Issue.

AB Is-oxazoles (I, R1 = H, Ac, CN, Me, Et, CO2Et, R2 = H, Me, NH2, Ph, pyridyl, iso-Bu, Et) and isoxazolines (II, R1 = H, Me, R2 = H, Me, CH2Ph, CO2Et, Et, R3 = Et, Ph, H, Me, etc., R4 = H, CH2Cl, CH2CN, CO2Et, etc.; III, R1 = 1-pyrrolidinyl, morpholino, piperidino, NEt2) were prepared by treatment of either 5-nitro-2-furohydroxamoyl halide in the presence of base or of 5-nitrofuronitrile oxide with olefins. Dihydro compds. (II, III) were treated with acid to give I. Thus, treatment of 5-nitro-2-furohydroxamoyl chloride and 1-piperidinocyclohexene with Et3N gave III (R1 = piperidino) (IV). IV at min. inhibitory concentration 0.01-10 .mu.g/ml was active against, e.g., Mycobacterium tuberculosis, Staphylococcus aureus, and Trichomonas vaginalis. About 75 addnl. I, II, and III were prepared similarly. Antimicrobial data for 21 addnl. I, II, and III were given.

ST antibacterial nitrofuryl isoxazoline; antiprotozoal nitrofuryl isoxazoline; furan nitro isoxazolyl antibacterial

IT Bactericides, Disinfectants and Antiseptics  
 Protozoacides

(nitrofurylisoxazolidines)

IT 7194-20-9P	7194-23-2P	7197-35-5P	7204-88-8P	14730-42-8P
14730-43-9P	14730-45-1P	14730-46-2P	14730-48-4P	
14730-49-5P	14730-50-8P	14730-52-0P	14734-52-2P	14734-55-5P
14734-56-6P	14734-57-7P	14734-58-8P	14734-59-9P	14734-60-2P
14775-77-0P	14775-78-1P	14775-79-2P	14775-81-6P	15154-19-5P
15381-96-1P	15382-00-0P	15427-09-5P	17819-27-1P	17960-17-7P
17960-18-8P	17960-19-9P	17960-21-3P	17960-25-7P	21694-00-8P
21694-05-3P	21706-48-9P	21706-49-0P	21706-51-4P	21706-53-6P
21706-54-7P	21706-56-9P	24247-97-0P	24247-98-1P	
24248-00-8P	24970-57-8P	24970-60-3P	24970-61-4P	24970-65-8P
24970-70-5P	24970-72-7P	24970-73-8P	24970-76-1P	24970-78-3P
24974-68-3P	25068-89-7P	26132-60-5P	36241-65-3P	36241-95-9P
36241-98-2P	36241-99-3P	36242-00-9P	36242-01-0P	

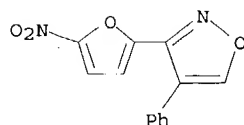
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 14730-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 14730-48-4 HCAPLUS

CN Isoxazole, 3-(5-nitro-2-furanyl)-4-phenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 56 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1971:125181 HCAPLUS  
 DN 74:125181  
 ED Entered STN: 12 May 1984  
 TI Hypotensive 3-isopropyltyrosine and 3-isopropyl-.alpha.-alkyltyrosines  
 IN Hansen, Holger Victor; Meltzer, Robert I.  
 PA Warner-Lambert Pharmaceutical Co.  
 SO U.S., 6 pp.  
 CODEN: USXXAM

DT Patent  
 LA English  
 IC C07C

NCL 260519000  
 CC 25 (Noncondensed Aromatic Compounds)  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3544623	A	19701201	US 1966-550918	19660518 <--
PRAI US 1966-550918		19660518 <--		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3544623	IC	C07C
	NCL	260519000

GI For diagram(s), see printed CA Issue.

AB The title compds. I and II, resp., where R = H or Me, were prepared by 2 procedures: (1) 1-isopropyl-2-alkoxybenzene with Zn(CN)2 in the presence of HCl and AlCl3 gave 3-isopropyl-4-alkoxybenzaldehyde (III). III with hippuric acid in the presence of NaHCO3 suspended in Ac2O gave 4-(3-isopropyl-4-alkoxybenzylidene)-2-phenyloxazol-5-one (IV) which was hydrolyzed with NaOH to 2-benzamido-3-(3-isopropyl-4-alkoxyphenyl)acrylic acid (V) and then hydrogenated (Pd/C) to the propionic acid (VI). VI with HCl gave an alkoxytyrosine which was refluxed with HBr to give I.HBr. In procedure (2), III was reduced by KBH4 to give the benzyl alc. which was converted to the cyanide. Treatment of the cyanide with a lower carboxylic acid alkyl ester in the presence of NaOEt gave the 1-cyanopropanone. After removal of the CN by HCl, it was treated with KCN and (NH4)2CO3 to give the hydantoin (VII). Further treatment with NaOH followed by HBr gave II.HBr. I and II inhibit the action of tyrosine hydroxylase and are useful in the treatment of other ailments resulting from excess amts. of sympathomimetic amines.

ST hypotensive tyrosine isopropyl alkyl

IT 31816-28-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hypotensive activity)

IT 31816-25-8P 31816-26-9P 31816-27-0P 31816-29-2P 31816-30-5P  
 31816-31-6P 31816-32-7P 31816-33-8P 31816-34-9P 31825-29-3P  
 31825-30-6P 31825-31-7P 31859-25-3P 33537-78-9P

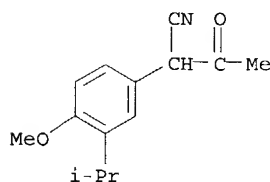
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 31816-30-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 31816-30-5 HCAPLUS

CN Acetoacetonitrile, 2-(4-methoxy-m-cumenyl)- (8CI) (CA INDEX NAME)



L28 ANSWER 57 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1971:88683 HCAPLUS

DN 74:88683

ED Entered STN: 12 May 1984

TI Light-sensitive diazotype material comprising aryl-substituted acylacetoneitriles or their ester or amide derivatives as coupling components

IN Sheehan, John M.

PA Tecnifax Corp.

SO U.S., 5 pp.

CODEN: USXXAM

DT Patent

LA English

IC G03C

NCL 096091000

CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3558318	A	19710126	US 1968-745697	19680718 <--
PRAI US 1968-745697		19680718 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3558318	IC	G03C
	NCL	096091000

AB The title compns. contain a mixture of a light-sensitive diazonium compound such as 3,4-Me(EtNH)C<sub>6</sub>H<sub>3</sub>N<sub>2</sub>+PF<sub>6</sub>- (I) and a coupler ArCH(COR) x (II), where R is Me or Ph and X is CN, CO<sub>2</sub>R<sub>1</sub> or CONH<sub>2</sub>. II (X = CN), prepared from ArCH<sub>2</sub>CN and RCO<sub>2</sub>Et in the presence of Na, are converted to II (X = CO<sub>2</sub>Et) by the action of dry HCl in EtOH, and into II (X = CONH<sub>2</sub>) by the action of BF<sub>3</sub> in HOAc.

ST diazotype light sensitive compds; light sensitive diazonium compds; diazonium light sensitive compds; nitrile azo coupling components; acetonitriles azo coupling components

IT Diazo process

(couplers for, phenylacetoacetic acid derivs. as)

IT 4433-77-6P 4468-48-8P 5219-07-8P 5413-05-8P

5415-07-6P 31573-38-3P 63895-78-3P

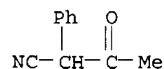
RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)

IT 4468-48-8P

RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)

RN 4468-48-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl- (9CI) (CA INDEX NAME)



L28 ANSWER 58 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1969:461400 HCAPLUS

DN 71:61400

ED Entered STN: 12 May 1984

TI 3,4-Dihydro-2H-1,3-benzoxazin-2-ones

IN Shavel, John Jr.; Bobowski, George

PA Warner-Lambert Pharmaceutical Co.

SO U.S., 11 pp.

CODEN: USXXAM

DT Patent

LA English

IC C07D; A61K

NCL 260244000

CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3446804	A	19690527	US 1965-504142	19651023 <--
PRAI US 1965-504142		19651023 <--		

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES  
 -----  
 US 3446804 IC C07DIC A61K  
 NCL 260244000

GI For diagram(s), see printed CA Issue.

AB The title compds. (I), useful as antiinflammatory agents, were made by treating 3,4-dihydro-4-hydroxy-2H-1,3-benzoxazin-2-one (prepared according to R. E. Strube, et al., 1964) with R<sup>2</sup>H. Thus, 6 g. 3,4-dihydro-4-hydroxy-3-methyl-2H-1,3-benzoxazin-2-one and 5.25 g. benzenesulfonamide in 100 ml. C<sub>6</sub>H<sub>6</sub> was refluxed for 2 hrs., while 0.6 ml. H<sub>2</sub>O was collected in a Dean-Stark trap, to give 9.2 g. 4-phenylsulfonamido-3,4-dihydro-3-methyl-2H-1,3-benzoxazin-2-one, m. 203-4.5.degree. (EtOAc) (decomposition). Similarly prepared were the following (I) (R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>, and m.p. given): Me, 4,4-dimethyl-2,6-dioxocyclohexyl, H, 196-7.degree. (decomposition); Me, Ac<sub>2</sub>CH, H, 136-8.degree.; Me, AcCHCO<sub>2</sub>Et, H, 140-1.degree.; Me, 2,5-dioxo-1-pyrrolidinyl, H, 182-3.degree.; Me, 5-methyl-2-furyl, H, 130-1.5.degree.; Me, 2-furyl, H, 123-4.degree.; Me, CH<sub>2</sub>Ac, H, 95-6.5.degree.; Me, CH<sub>2</sub>COAc, H, 141-3.degree.; Me, CH<sub>2</sub>COCH<sub>2</sub>Cl, H, 162-4.degree. (decomposition); Me, AcC(CN)Ph, H, 160-1.degree.; Me, Me, CH<sub>2</sub>COC<sub>6</sub>H<sub>4</sub>Me-p, H, 153-4.degree. (decomposition); Me, 2-thienyl, H, 136-7.degree. (decomposition); Me, C<sub>6</sub>H<sub>4</sub>OH-p, H, 219-20.degree.; Me, AcCHBz, H, 163-5.degree. (decomposition); Me, MeNCONHMe, H, 156-7.degree. (decomposition); Me, NHCO<sub>2</sub>Et, H, 167-8.degree.; Me, NHCO<sub>2</sub>Et, 6-Cl, 191-2.degree. (decomposition); Me, NHCO<sub>2</sub>Et, 7-MeNHCO<sub>2</sub>, 175-8.degree. (decomposition); Me, NHCO<sub>2</sub>Et, 8-MeO, 166-7.degree.; CH<sub>2</sub>CH:CH<sub>2</sub>, NHCO<sub>2</sub>Et, H, 113-14.degree.; CH<sub>2</sub>CH:CH<sub>2</sub>, NHCO<sub>2</sub>Et, 6-Cl, 156-8.degree. (decomposition); CH<sub>2</sub>CH:CH<sub>2</sub>, NHCO<sub>2</sub>Et, 8-MeO, 127.5-29.degree.; CH<sub>2</sub>CH:CH<sub>2</sub>, NHCO<sub>2</sub>Et, 7-CH<sub>2</sub>:CHCH<sub>2</sub>NHCO<sub>2</sub>, 155.5-7.0.degree.; CH<sub>2</sub>CH:CH<sub>2</sub>, NHCO<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl, 8-MeO, 127-8.degree.; Me, MeNCO<sub>2</sub>Et, 6-Cl, 96-7.degree.; CH<sub>2</sub>CH:CH<sub>2</sub>, MeNCONHMe, H, 148-9.degree.; Me, MeO, 8-MeO, 88-90.degree.; and Me, NHCONH<sub>2</sub>, H, 203-4.degree. (decomposition).

ST oxazinones dihydro; benzoxazinones; antiinflammatory agents

IT Inflammation  
 (inhibitors of, dihydrobenzoxazinones as)

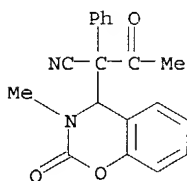
IT 7646-09-5P 7646-10-8P 7646-11-9P 7646-13-1P 7646-14-2P  
 7646-15-3P 7646-16-4P 7646-17-5P 7646-18-6P 7646-19-7P  
 7646-21-1P 7646-22-2P 7646-23-3P 7646-24-4P 7646-25-5P  
 7646-26-6P 7646-27-7P 7646-28-8P 7678-08-2P 7678-09-3P  
 7687-92-5P 7687-94-7P 7688-15-5P 23240-88-2P 23241-00-1P  
 23241-01-2P 23241-02-3P 23241-03-4P 23241-04-5P 23241-06-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 23240-88-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 23240-88-2 HCAPLUS

CN 2H-1,3-Benzoxazine-4-acetonitrile, .alpha.-acetyl-3,4-dihydro-3-methyl-2-oxo-.alpha.-phenyl- (8CI) (CA INDEX NAME)



L28 ANSWER 59 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1969:3558 HCAPLUS  
 DN 70:3558  
 ED Entered STN: 12 May 1984  
 TI Ketones and aldehydes  
 IN Landis, Phillips S.  
 PA Mobil Oil Corp.  
 SO U.S., 5 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 NCL 260094900  
 CC 25 (Noncondensed Aromatic Compounds)  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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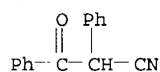
PI US 3382226 A 19680507 US 1965-440618 19650317 <--  
 PRAI US 1965-440618 19650317 <--

## CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

US 3382226 NCL 260094900

AB RR1R2CCR3R4COR5 are prepared from RR1R2CH and R3R4C:C(OR6)R5. Thus, a mixture of 1.07 g. .alpha.-methoxystyrene (I) and 8.45 g. PhMe was sealed under N and heated at 250.degree. for 24 hrs. Methane gas was released and the starting material and by-products were distilled. The residue was digested with 15 ml. methanol to give .beta.-penylpropionophenone, m. 71-3.degree.. Similarly prepared were: .alpha.-(tetrahydronaphthyl)-acetophenone, b0.05 190-5.degree., 2-(1,2,3,4,5,6-pentamethylbenzyl)-cyclohexan-1-one, m. 121-3.degree., and .beta.-benzoyl-.alpha.-phenylacetoneitrile, m. 120-2.degree.. Similar reactions were carried out (reactants and m.p. of products given): hexamethylbenzene and I, 3 products m. 108-28.degree., 115-65.degree., and 124-6.degree.; hexadecane and I, 210-12.degree.; polyethylene (m. 150.degree.) and I, -; hexaethylbenzene, I, -.  
 ST acetophenones; propionophenones  
 IT 1083-30-3P 5415-07-6P 20805-73-6P 26898-23-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 5415-07-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 5415-07-6 HCAPLUS  
 CN Benzenepropanenitrile, .beta.-oxo-.alpha.-phenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 60 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1968:96127 HCAPLUS

DN 68:96127

ED Entered STN: 12 May 1984

TI L-.alpha.-Methyl-3,4-dihydroxyphenylalanine, an antihypertensive agent

IN Reinhold, Donald F.; Sletzing, Meyer

PA Merck and Co., Inc.

SO U.S., 10 pp.

CODEN: USXXAM

DT Patent

LA English

NCL 167065000

CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3344023		19670926	US	19600824 <--

## CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

US 3344023 NCL 167065000

AB The title compound (L-I) was compared with DL-I and D-I in humans as an antihypertensive. To a solution of 74.3 g. 3,4,5-trimethoxybenzaldehyde in 121 ml. PhMe were added 50.1 g. nitroethane, 3.03 ml. BuNH2, and 3.60 ml. HOAc. The mixture was refluxed, azeotropically removing H2O, and excess reactants removed. Trituration with Skellysolve B gave 1-(2-nitropropen-1-yl)-3,4,5-trimethoxybenzene (II). II (96 g./50 ml. PhMe) was added to 137.4 g. 40-Mesh Fe, 2.75 g. FeCl3.H2O, and 172 ml. H2O. This was refluxed with dropwise addition of 248 ml. HCl, refluxed several more hrs. and cooled. Siliceous filter aid was added, filtered off, and washed with C6H6. The aqueous layer was acidified to pH 2 and extracted with C6H6. The combined C6H6 was extracted with H2O, stirred 1 hr. with 10% NaHSO3, washed with H2O, dried, and evaporated to give 1-(3,4,5-trimethoxyphenyl)-2-propanone (III), an oil. Similarly prepared were 1-(3,4-dimethoxyphenyl)-2-propanone (IV), 1-(3-methoxyphenyl)-2-propanone (V) and 1-(4-hydroxy-3-methoxyphenyl)-2-propanone. A solution of 88.5 g. 3,4-dimethoxyphenylacetoneitrile in 198 ml. Et propionate was added to 34.5 g. Na in 400 ml. absolute EtOH containing 2% C6H6 and refluxed 4 hrs. Filtration, washing with 200 ml. EtOAc and 200 ml. Et2O, dissoln. in 1200 ml. H2O, cooling to 10.degree., slow addition of 115 ml. HOAc, extraction with Et2O, and drying and concentration of the Et2O yielded 1-cyano-1-(3,4-dimethoxyphenyl)-2-

butanone (VI), an orange oil. VI was slowly added to 250 ml. H<sub>2</sub>SO<sub>4</sub> + 60 ml. H<sub>2</sub>O at 0-5.degree., heated at 80.degree. for 10 min., at 90.degree. for 3 hrs. and cooled. This was extracted with Et<sub>2</sub>O, the extract was washed with 100 ml. 5% NaHCO<sub>3</sub> and 100 ml. H<sub>2</sub>O, dried, and concentrated to give liquid 1-(3,4-dimethoxyphenyl)-2-butanone. Keeping the temperature at 25-60.degree., 48 g. III in 484 ml. EtOH was added to 165 g. (NH<sub>4</sub>)<sub>2</sub>CO<sub>3</sub> + 35.4 g. KCN in 484 ml. H<sub>2</sub>O. Reaction at 55-60.degree. for 18 hrs. and concentration to 1/3 volume in vacuo gave 5-methyl-5-(3,4,5-trimethoxybenzyl)hydantoin (VII), recrystd. from 50% aqueous EtOH. Reaction of 10 g. VII, 45 g. Ba(OH)<sub>2</sub>·8H<sub>2</sub>O, and 226 ml. H<sub>2</sub>O in an autoclave at 150.degree., treatment with CO<sub>2</sub> gas at 50.degree., filtration, and washing of the BaCO<sub>3</sub> precipitate with hot H<sub>2</sub>O, pH adjustment to 6.4 with 2N H<sub>2</sub>SO<sub>4</sub> of the combined aqueous portions, hot filtration through siliceous filter aid, and evaporation to dryness gave .alpha.-methyl-.beta.-(3,4,5-trimethoxyphenyl)alanine (VIII). A mixture of 9.15 g. VIII in 124 ml. 48% HBr was refluxed under N for 5 hrs., concentrated in vacuo, flushed with tert-BuOH and H<sub>2</sub>O, put on an Amberlite IR-45 hydroxide cycle column, eluted with 800 ml. H<sub>2</sub>O, and concentrated to 20 ml. in vacuo to precipitate .alpha.-methyl-.beta.-(3,4,5-trihydroxyphenyl)alanine (IX). Similarly prepared was .alpha.-ethyl-.beta.-(3,4,5-trihydroxyphenyl)alanine; similarly were prepared from IV, .alpha.-methyl-.beta.-(3,4-dihydroxyphenyl)alanine (X), and from V, .alpha.-methyl-.beta.-(3-hydroxyphenyl)alanine. At 10-20.degree. a suspension of 25 g. IX + 250 ml. MeOH was saturated with HCl gas, refluxed for 3 hrs., and allowed to stand 18 hrs. Working under N, repeated in vacuo removal of MeOH and MeOH addition followed by dissoln. in H<sub>2</sub>O, and precipitation by NH<sub>4</sub>OH addition to pH 8.5 yielded the Me ester of IX. To a mixture of boiled and then cooled 5.73 g. NaOH + 10 ml. H<sub>2</sub>O was added 10 g. X and 50 g. ice-H<sub>2</sub>O. Addition of 11.13 ml. Ac<sub>2</sub>O, reaction at 0.degree. for 1 hr., filtration, washing with 9:1 iso-PrOH-H<sub>2</sub>O, dissoln. in a hot mixture of 100 ml. iso-PrOH + 25 ml. H<sub>2</sub>O, filtration, and cooling precipitated .alpha.-methyl-.beta.-(3,4-diacetoxyphenyl)alanine. Reaction of 25 g. X, 100 ml. Ac<sub>2</sub>O, and 75 ml. C<sub>5</sub>H<sub>5</sub>N under N at 90.degree. for 2 hrs., standing overnight at 25.degree., concentration in vacuo, stirring with ice-H<sub>2</sub>O, and acidification with 2.5N HCl precipitated N-acetyl-.alpha.-methyl-.beta.-(3,4-diacetoxyphenyl)alanine (XI). Similarly prepared was N-acetyl-.alpha.-methyl-.beta.-(3,4-dimethoxyphenyl)alanine (XII). A slurry of 2.1 g. XII in 4 ml. MeOH and 0.91 g. L-.alpha.-phenylethylamine (L-XIII) in 1 ml. MeOH was prepared, heated to reflux, diluted with 10 ml. MeOH, and refluxed until complete solution occurred. This was filtered through diatomaceous earth, the filter cake washed with 10 ml. H<sub>2</sub>O, the MeOH distilled, the solution cooled to 60.degree., seeded with L-XII.L-XIII salt, cooled to 25.degree., aged at 8.degree. for 18 hrs., swirled, and again aged at 80.degree. for 24 hrs. The crude salt was filtered off, washed with cold H<sub>2</sub>O, and dried in vacuo at 56.degree., [.alpha.]D 55.degree. (c 1, MeOH). Recrystn. from H<sub>2</sub>O gave pure L-N-acetyl-.alpha.-methyl-.beta.-(3,4-dimethoxyphenyl)alanine L-.alpha.-phenyl-ethylamine, [.alpha.]D 69.degree.. A solution of 33.2 g. D-XIII in 50 ml. MeOH was added to slurry of 77 g. XII in 200 ml. MeOH. Addition of 1 l. H<sub>2</sub>O, removing the MeOH in vacuo at 50-60.degree., heating to 90.degree., filtration through diatomaceous earth, seeding with D-XII.D-XIII salt, cooling as above, filtration, H<sub>2</sub>O washing, and drying over P<sub>2</sub>O<sub>5</sub> yielded D-XII.D-XIII salt, [.alpha.]D -59.degree. (c 1, MeOH). The mother liquors + 50 ml. 2.5N NaOH were extracted with CHCl<sub>3</sub>. Addition of 15 ml. HOAc to the aqueous phase and aging at 8.degree. for 19 hrs. yielded crude L-XII, [.alpha.]D -23.degree.. Treatment with L-XIII and recrystn. from aqueous MeOH gave pure L-XII.L-XIII, [.alpha.]D 68.degree.. Treatment of 25 g. L-XII.L-XIII in 100 ml. H<sub>2</sub>O with 27.5 ml. 2.5N NaOH, extraction of the L-XIII with CHCl<sub>3</sub>, and acidification with HCl yielded L-XII, [.alpha.]D -56.degree.. Treatment of L-XII with 48% HBr (as previously) gave L-X, [.alpha.]D -4 .+- .2.degree. (c 1, N HCl). The Et ester of L-X had [.alpha.]D -10.degree. (c 1, N HCl). The L-XI quinone salt had [.alpha.]D 23D -72.5.degree. (c 1, 96% EtOH). Similarly prepared was L-.alpha.-methyl-m-tyrosine, [.alpha.]D -2 .+- .1.degree. (c 1, 1N HCl). An initial blood pressure of 200 was lowered to 140 with 4.5 g./day DL-I, raised to 200 with 4.5 g./day D-I, and lowered to 130 with 2.25 g./day L-I. Similarly, tests with another subject went from 150 to 110 to 150-160 to 100-110.

ST ANTIHYPERTENSIVE DIHYDROXY PHENYL; PHENYLALANINES ANTIHYPERTENSIVE;  
DIHYDROXY; DIHYDROXY PHENYLALANINES; ALANINES

IT Hypertension

(3-(3,4-dihydroxyphenyl)-2-methyl-L-alanine in treatment of)

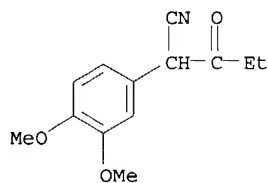
IT 55-40-3 2799-15-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(as antihypertensive agent)

IT 555-30-6P

RL: PREP (Preparation)  
(manufacture of, as antihypertensive agent)

IT 831-74-3P 884-06-0P 976-34-1P 1230-40-6P 5389-29-7P 5556-76-3P  
5934-66-7P 6014-30-8P 6892-05-3P 16603-18-2P 16825-27-7P  
17762-33-3P 17762-35-5P 17772-80-4P 17772-81-5P  
17772-83-7P 17772-88-2P 17772-92-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
IT 17762-33-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 17762-33-3 HCAPLUS  
CN Veratronitrile, .alpha.-propionyl- (8CI) (CA INDEX NAME)



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